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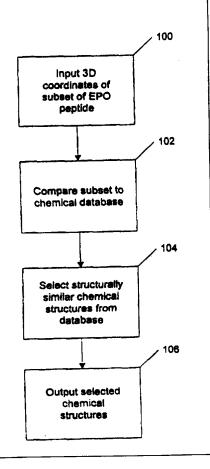
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(54) Title: SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN

(57) Abstract

The invention features computer-assisted methods (100, 102, 104, 106, 200, 202, 204) for identifying molecules which will bind to the EPO receptor and act as an erythropoietin (EPO) mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more *in vitro* or *in vivo* biological assays of EPO activity.



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SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN

BACKGROUND OF THE INVENTION

1. Field of the Invention

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This invention relates to computer-assisted methods for identifying and designing small molecule mimetics of erythropoietin.

2. Description of Related Art

Erythropoietin (EPO) is the primary regulator of the proliferation and differentiation of immature erythroid cells. EPO is produced in the fetal liver and in the adult kidney in response to hypoxia (low oxygen levels in blood or tissue). It circulates in the blood stream where it targets the EPO receptor (EPOR) on committed progenitor cells in the bone marrow and other hematopoietic tissues. Recombinant human erythropoietin (rHuEPO) is widely used in therapy of patients with anaemia due to chronic renal failure, cancer chemotherapy and AZT treatment.

The EPO receptor belongs to the cytokine receptor superfamily which includes receptors for other hematopoietic growth factors such as interleukins (ILs), colony stimulating factors (CSFs) as well as growth hormone prolactin and ciliary neurotrophic factor (CNTF). The structural architecture of this family of receptors consists of three modules: a ligand binding extracellular domain, a short trans membrane region and a large cytoplasmic domain. It has been proposed that the extracellular domain of this superfamily comprises two discrete domains each containing approximately 100 residues that fold into a sandwich consisting of 7 antiparallel β-strands with the topology of an Ig constant domain. Members of the family share two characteristic motifs in their extracellular domain: a pair of conserved disulfide bridges in the N-terminal domain, and a WSXWS box (where X is any amino acid residue) in the C-terminal domain. For most members of this receptor superfamily, oligomerization of one or more polypeptide chains

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is essential for forming high affinity receptor complexes. A homodimer complex has been demonstrated to be the active form of hGHR and a similar model has been suggested for G-CSF, prolactin and EPO receptors.

Erythropoietin induces dimerization of two EPO receptor molecules, which results in subsequent phosphorylation of the cytoplasmic domains by the association with two tyrosine kinase (JAK2) molecules to initiate a cascade of events that leads to the relevant biological.

Given the importance of erythropoietin, it would be very desirable to be able to identify molecules capable of binding the EPO receptor and eliciting the response normally elicited by EPO.

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SUMMARY OF THE INVENTION

The invention features methods for identifying molecules which will bind to the EPO receptor and act as a EPO mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more *in vitro* or *in vivo* biological assays of EPO activity. Preferred mimetics are molecules lacking peptide bonds, i.e., are non peptidic mimetics. Preferred peptide mimetics have 15 or fewer, more preferably 10 or fewer amino acids.

The methods of the invention entail identification and design of molecules having a particular structure. The methods rely on the use of precise structural information derived from x-ray crystallographic studies of the extracellular domain of EPO receptor (amino acids 1 to 225) complexed with a peptide, EMP1 (EPO Mimetic Peptide 1; described below), which acts as an EPO mimetic. This crystallographic data permits the identification of atoms in the peptide mimetic that are important for EPO receptor binding and dimerization. More importantly, this data defines a three dimensional array of the important contact atoms. Other molecules which include a portion in which the atoms have a similar three dimensional arrangement similar to some or all of these contact atoms are likely to be capable of acting as an EPO mimetic. Moreover, one can use the structural information to design or identify molecules having even more EPO activity than the peptide mimetic described herein.

The details of the preferred embodiment of the present invention are set forth in the accompanying drawings and the description below. Once the details of the invention are known, numerous additional innovations and changes will become obvious to one skilled in the art.

BRIEF DESCRIPTION OF THE DRAWINGS

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system.

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system.

Like reference numbers and designations in the various drawings indicate like elements.

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DETAILED DESCRIPTION OF THE INVENTION

Throughout this description, the preferred embodiment and examples shown should be considered as exemplars, rather than as limitations on the present invention.

Described below is the crystal structure of a small peptide mimetic of EPO bound to an EMP1 **EPO** receptor. The peptide, extracellular portion of the (GGTYSCHFGPLTWVCKPQGG; SEQ ID NO:1), is characterized by an intramolecular disulfide bridge. Several lines of evidence suggest that EMP1 can act as an EPO mimetic. For example, EMP1 competes with EPO in receptor binding assays and induces cellular proliferation of cell lines engineered to be responsive to EPO. Both EPO and peptide induce a similar cascade of phosphorylation events and cell cycle progression in EPO responsive cells. Furhter, EMP1 demonstrates significant erythropoietic effects in mice as monitored by two different in vivo assays of nascent red blood cell production. This data, when combined, strongly supports the notion that the peptide ligand, which has a sequence unrelated to that of EPO, is capable of binding to and inducing an agonist conformation or assembly of EPO receptor.

Design of small molecule mimetics

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The structure of the EMP1 dimer demonstrates that a molecule substantially smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide is assumed to have a substantially smaller contact interface with the receptor than its natural hormone. The binding determinants in the EPO receptor form an almost flat surface which is mainly hydrophobic in nature, without any cavities or charged residues that may help in design of a small molecule ligand to interact with the receptor.

This simplified framework of interactions revealed by the structural data presented herein can be used to identify additional EPO mimetics. The atoms of EMP1 which are important for binding to the EPO receptor and forming dimeric EPO receptor include those involved in the contact between the EMP1 (peptide) and EBP (EPO receptor) and

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those involved in contacts between the two EMP1 molecules in the dimeric complex (peptide-peptide contacts). In addition to the contacts listed in Table 2, the following EMP1-EMP1 hydrophobic contacts are significant: Tyr^{P4}, Cys^{P6}, Phe^{P8}, Trp^{P13}, and Cys^{P15} in each peptide. The following EMP1-EBP hydrophobic interactions are also significant: Tyr^{P4}, Phe^{P8}, and Trp^{P13} in each peptide. It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a mimetic. In fact, it is only those few atoms which actually from important contacts with the EPO receptor which are likely to be important for mimetic activity. Those skilled in the art will be able to identify these important atoms based on the model of the dimeric EMP1-EPO complex which can be constructed using the structural data herein.

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Preferred mimetics will include atoms at postions similar to those of the EPO receptor contacting atoms of EMP1. Even more preferred mimetics will be structurally similar to the dimer of EMP1 found in the structure described below. This is because the dimerization of EMP1 is an important factor in the diemerization of the EPO receptor.

The methods of the invention employ a computer-based methods for identifying compounds having a desired structure. More specifically, the invention uses the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the human EPO receptor, to determine peptide and non-peptide mimetic candidates by means of computer methods.

These computer-based methods fall into two broad classes: database methods and *de novo* design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional (*i.e.*, sequence)

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data. In de novo design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, e.g., data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atom-by-atom manner or by assembling stored small molecular fragments.

The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally relevant portion of the compound of interest. For drugs, the functionally relevant portion is referred to a pharmacophore. A pharmacophore then is an arrangement of structural features and functional groups important for biological activity, *e.g.*, EPO activity.

Not all identified compounds having the desired pharmacophore will act as an EPO mimetic. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds which must be tested to identify an actual mimetic.

Dimerization of the EPO receptor is important for activity. Accordingly, preferred mimetics will be based on the structure of the EMP1 dimer as it is bound to the EPO receptor dimer. Thus, preferred mimetics have include important contacts from both of the RWJ 61233 peptides present in the structure described below. Such mimetics will favor dimerization of the EPO receptor.

Programs suitable for generating predicted three-dimensional structures from two-dimensional data include: Concord (Tripos Associated, St. Louis, MO), 3-D Builder (Chemical Design Ltd., Oxford, U.K.), Catalyst (Bio-CAD Corp., Mountain View, CA), and Daylight (Abbott Laboratories, Abbott Park, IL).

Programs suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore include: MACCS-3D and ISIS/3D (Molecular Design Ltd., San Leandro, CA), ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.), and Sybyl/3DB Unity (Tripos Associates, St. Louis, MO).

Programs suitable for pharmacophore selection and design include: DISCO (Abbott Laboratories, Abbott Park, IL), Catalyst (Bio-CAD Corp., Mountain View, CA), and ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.).

Databases of chemical structures are available from Cambridge Crystallographic Data Centre (Cambridge, U.K.) and Chemical Abstracts Service (Columbus, OH).

De novo design programs include Ludi (Biosym Technologies Inc., San Diego, CA) and Aladdin (Daylight Chemical Information Systems, Irvine CA).

Those skilled in the art will recognize that the design of a mimetic may require slight structural alteration or adjustment of a chemical structure designed or identified using the methods of the invention.

- In general, chemical compounds identified or designed using the methods of the invention can be sythesized chemically and then tested for EPO activity using any of the methods described below. The methods of the invention are particularly useful because they can be used to greatly decrease the number potential mimetics which must be screened for EPO activity.
- The invention may be implemented in hardware or software, or a combination of both. However, preferably, the invention is implemented in computer programs executing on programmable computers each comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions

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described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The inventive system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

- (1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 100);
- comparing, using the processor, the criteria data set to a computer database of chemical structures stored in the computer data storage system (STEP 102);

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- (3) selecting from the database, using a program suitable for searching threedimensional databases to identify molecules bearing a desired pharmacophore (such as those described above or equivalents), chemical structures having a portion that is structurally similar to the criteria data set (STEP 104);
- (4) outputting to an output device the selected chemical structures having a portion similar to the criteria data set (STEP 106).

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

- (1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 200);
- (2) constructing, using a program suitable for generating chemical structure models (such as those described above or equivalents), a model of a chemical structure having a portion that is structurally similar to the criteria data set (STEP 202),
- (3) outputting to the output device the constructed model (STEP 204).

20 Confirmation of Biological Activity

In order to determine whether a molecule identified using the methods of the invention can act as an EPO mimetic, one or more *in vitro* or *in vivo* assays of EPO activity should be performed. For example, mimetic molecules should be able to stimulate proliferation of TF-1 cells (Kitamura et al., J. Cell Physiol. 140:323, 1985) or B6Sut cells (Greenberger et al., Proc. Natl. Acad. Sci. USA 80:2931, 1983), but preferably do not stimulate proliferation of cells which do not bear the EPO receptor. Thus, preferred mimetics do not stimulate proliferation of Mo7e cells (Avanzi et al., Br. J. Haematol. 69:359, 1988).

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Potential mimetics can also be tested in a murine model of erythropoiesis. In this assay a potential mimetic is administered to normal mice which express endogenous basal levels of EPO. Reticulocytes are counted, preferably by flow cytometry, to determine whether the candidate mimetic increases reticulocyte levels. An increase in reticulocyte levels indicates that the candidate mimetic is stimulating erythropoiesis. Because the mice used in this assay already express EPO, this assay may be relatively insensitive. As an alternative, candidate mimetics can be assayed in the exhypoxic-polycythemic mouse bioassay. In this assay polycythemia is induced by conditioning mice in a hypobaric chamber to reduce endogenous EPO levels. A potential EPO mimetic can be administered to a conditioned mouse. Incorporation of ⁵⁹Fe into blood serves as a measure of erythropoiesis. This erythropoiesis can be attributed to the candidate mimetic.

The assays described above are examples of suitable assays. Other assays for EPO activity known to those skilled in the art are also useful.

In order to determine the biological activity of a candidate mimetic it is preferable to measure biological activity at several concentrations of candidate mimetic. The activity at a given concentration of candidate mimetic can be compared to the activity of EPO itself.

Structural Data

The coordinates for amino acids 1 to 225 of the human EPO receptor bound to peptide EMP1 are presented in the attached appendix in standard Brookhaven database format. Also included in this appendix is a list of van der Waals interactions. These coordinates can be used in the design and identification of EPO mimetics according to the methods of the invention.

Structure of EBP-EMP1 Complex

The extracellular fragment of human EPO receptor (EPO binding protein, EBP), consisting of residues 1-225, was expressed in <u>Escherichia coli</u> and purified as described

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(Johnson et al., Protein Express. Purif. 7:104, 1996). Rhomboidal-shaped crystals of an EBP complex with EMP1 were obtained in orthorhombic space group P2₁2₁2₁, with cell parameters a=59.2Å, b=75.5Å, c=132.2Å, with two EBP and two peptide molecules in the asymmetric unit and a V_M=2.8 Å³/dalton (Matthews, J. Mol. Biol. 33:491, 1968). The crystal structure was determined by multiple isomorphous replacement (MIR) using two heavy atom derivatives (Table 1). Residues 1-2 and 19-20 of each peptide as well as residues 1-9, 21-23, 164-166, 221-225 of receptor molecule I, and residues 1-9, 21-23, 133-135, 221-225 of receptor molecule II had poor or no electron density and are excluded from the structure analyses

An important break in the electron density that affects the structure interpretation occurs for the three residues (Arg²¹ -Gly²² -Pro²³) that link the amino terminal α -helix to the first β-strand in D1 of both receptor molecules. A molecular packing diagram shows the proximity of a second non-crystallographically related dimer in the crystal that gives two possibilities of how this three-residue linker may be connected. The current choice of linker connectivity is based on a structure of another independent EBP-peptide complex at higher resolution (2.5 Å), which shares a similar molecular packing, but for which the electron density is clear for these three residues. At present there are no experimental data to verify whether this N-terminal \alpha-helix exists in solution or is a crystallization packing artifact. Notably, this helical region is not observed in the published structures of hGHbp (begins at residue 32; deVos et al., Science 255:306, 1992), PRLR (begins at residue 2, without any defined secondary structure until the first β-strand, residue 6; Somers et al., Nature 372:478, 1994), the INF-yRa (begins at residue 17; Walter et al., Nature 376:230, 1995) or the tissue factor (begins at residue 3 without any defined secondary structure until the first β-strand, residue 11; Muller et al., Nature 370:662, 1994).

The EBP monomer folds into two domains, D1 and D2, that form an L-shape with the long axis of each domain aligned at approximately 90° to each other; the overall molecular dimensions are 45 Å x 52 Å x 62 Å. The N-terminal domain (D1, residues 10-

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114) and C-terminal domain (D2, residues 119-220) are connected by a short four residue α-helix linker. Both domains are more closely related in overall topology to Fibronectin type-III (FBN-III) domains than to Ig domains (Bork et al., J. Mol. Biol., 242:309, 1994). The FBN-III fold is composed of two antiparallel β -pleated sheets, consisting of strands A, B, E and strands G, F, C and C', and is found in the two domains of the human growth hormone (de Vos et al., Science 255:306, 1992) and prolactin (Somers et al., Nature 372:478, 1994) receptors, the D1 and D2 domains of the α chain of interferon- γ receptor (IFN-γRα) (Walter et al., Nature 376:230, 1995), the D2 domain of CD4 (Wang et al, Nature 348:411, 1990; Ryu et al., Nature 348:419, 1990), the two domains of tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994), the third fibronectin-type repeat of tenacin (Leagy et al., Science 258:987, 1992) and the D2 domain of the chaperone protein PapD (Holmgren et al., Nature 342:248, 1989). The FBN-III topology differs from an Ig constant domain by a shift of strand D from one β sheet (strands A, B, E and D) to the other (strands G, F, C, C'), where it is defined as the C' strand. Superposition of equivalent β -sheet core residues of the D1 and D2 domains in EBP gives an r.m.s. deviation of 2.3 Å for 77 Ca pairs, which is significantly larger than the corresponding domain overlaps for hGHbp (1.1Å) and PRLR (0.8Å), and reflects a difference in the subclass of fold between the two EBP domains.

In D1, a short α -helix (residues 10-20), precedes the first β -sandwich that is better described as a hybrid of the FBN-III fold with an Ig fold (residues 24-114), rather than strict FBN-III topology. In this h-type fold (Wang et al., Nature 348:411, 1990; Ryu et al., Nature 348:419, 1990), the C' strand is long and interacts first with strand C and then switches to interact with strand E (where C' changes its designation to strand D) forming a four-on-four strand β -sandwich. D1 contains the two conserved disulfide bridges linking Cys ²⁸ (β A) to Cys ³⁸ (β B) and Cys ⁶⁷ (β C') to Cys ¹⁸ (β E). The number of residues between the cysteine pairs that form the two disulfide bridges are 9 and 15 for EBP, compared to 9 and 10 in both GHR and PRLR. The longer connection between strands C' and E enables the second half of strand C' to become strand D. This h-type topology is not found in either of the two s-type GHR domains. A potential glycoylation site exists

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on residue Asn^{52} which is located towards the end of the loop region connecting the βB and βC strands. Although Asn^{52} is not glycosylated in this bacterially expressed protein, an external cavity around the Asn^{52} side chain could easily accommodate a carbohydrate moiety.

A helical linker (residues 115-118) connects D1 to D2 (The φ, Ψ torsion angles for the interdomain helical linker for lle¹¹³, Asn¹¹⁶, Glu¹¹⁷ and Val¹⁸ are -50° -27°, -76°, -21°, -99°, 26°, and -151°, 38° respectively.) and has been observed in other members of this receptor family, hGHbp, PRLR, IFN-γRα and tissue factor. In EBP, the domain association is further restricted by a mixed assortment of hydrogen bonding, hydrophobic interactions and one salt bridge (between Arg³² and Asp¹²²) from 11 residues of D1 and 12 residues of D2 with a total buried surface [The molecular surface areas buried by interaction were calculated using the program MS (Connolly, J. Appl. Crystallog, 16:439, 1983) using a 1.7Å probe sphere and standard atomic radii (as described in Davies, et al, Ann. Rev. Biochem. 59:439, 1990). There may be some discrepancies between values reported here and other (deVos et al., Scince 255:306, 1992) published values due to use of a different algorithm (Connolly) vs. Lee et al., J. Mol. Biol., 55: 379, 1971) and probe radii. For clarity all values reported here have been calculated in the same way for better comparison between the receptors] of 950 Ų for the two domains.

D2 (residues 119-220) folds into the standard FBN-III (s-type) topology with one free cysteine and no disulfide bridges, consistent with GHR and PRLR that have three and two disulfide bridges, respectively, in D1 but none in D2. After the α -helix linker, D2 begins with an irregular coil (residues 118-126) that contains Pro^{124} which is conserved in the structures of hGHbp, PRLR, tissue factor and IFN γ -R α , and based on sequence alignment, in most class-1 and class-2 cytokine receptors (Bazan, Proc. Natl. Acad. Sci. USA 87:6934, 1990). This short coil ends with Gly¹²⁴ which has a positive ϕ (ϕ , $\Psi \approx 52^{\circ}$,40°) consistent with the equivalent Ala¹³⁶ and Ala¹⁰¹ torsion angles in hGHbp (ϕ , $\Psi \approx 63^{\circ}$,68°) and PRLR (ϕ , $\Psi \approx 58^{\circ}$,38°). The Pro¹²⁴ region forms an analogous extended bulge conformation adjacent and parallel to a corresponding bulge containing the

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WSXWS motif. The WSAWS sequence forms a modified wide β -bulge (Richardson, Adv. Prot. Chem. 34:167, 1981) and is located in an extended chain region immediately preceding the βG strand that would normally connect to the membrane spanning region of the EPOR.

The quaternary structure of the complex is composed of two peptides and two receptors that form a T-shapes assembly. A noncovalent peptide dimer interacts with two receptor molecules to generate an almost perfect 2-fold symmetrical arrangement. After superposition of D2 of the two EBP molecules in the dimer, the centers of mass of the two D1 domains are only 0.8 Å apart, sufficient to perturb perfect two-fold symmetry.

Separate superposition of the corresponding D1 and D2 of each receptor in the dimer results in r.m.s. deviations of 0.53 Å (105 D1 Cα pairs) and 0.47 Å (93 D2 Cα pairs).

The cyclic EMP1 contains a single disulfide bridge between Cys^{P6} and Cys^{P15}, which links two short β-strands (residues 4-7 and 13-16) that are connected by a slightly distorted type 1 β -turn [Pro^{P10} (i+1) and Leu^{P11} (i+2) of the β -turn have $\phi, \Psi \approx -62^{\circ}$, -38° and -99°, -60°, respectively. The carbonyl oxygen of LeuP11 has a hydrogen bond to EBP distorting the Ψ value from its normal 0°±30° (i+2) in a standard type I β -turn.] consisting of residues Gly^{P9}-Pro^{P10}-Leu^{P11}-Thr^{P12}. Each peptide has a very close association with its other peptide partner and buries 320 Å of its 1220 Å² molecular surface in this interaction (Connelly, J. Appl. Crystallog. 16:439, 1983; Davies et al., Ann. Rev. Biochem. 59:439, 1990; Richards, J. Mol. Biol. 55:379, 1971). Four hydrogen bonds between the mainchains of the two peptides results in formation of a four-stranded anti-parallel βpleated sheet (Table 2). Two symmetric hyrdophobic cores are assembled by peptide dimerization and are comprised of the disulfide bridges and the side chains of TyrP4, PheP2 and Trp^{P13}. The construction of each hydrophobic core resembles a box which places the aromatic rings of PheP8, TrpP13 and TyrP4 (from the other peptide) and the disulfide bridge (Cys^{P6}-Cys^{P15}) at the corners. The two glycine residues at either end of the peptide are not structured.

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The peptide dimer is embedded in a deep crevice between two EBP receptor molecules. A portion of each peptide monomer interacts with both receptor molecules. The binding sites of each EBP are practically identical due to the 2-fold symmetric interactions imposed on binding the peptide dimer. The four major contact areas on EBP come from segments on four loop regions (L1, L3, L5, L6) that connect strands A to B (L1 residues 33-34) and F to G (L6 residues 90-94) in D1 and strands B to C (L5 residues 148-153) and F to G (L6 residues 203-205) in D2. The total buried molecular surfaces in the peptide-EBP assembly are 840 Å² and 880 Å² for the two peptides and EBP's, respectively. The peptide-EBP interaction can be separated into distinct hydrophobic (67%) and polar (33%) areas. A hydrophobic core is formed between the peptide and receptor and comprises Phe93, Met150 and Phe205 from one EBP molecule and the peptide hydrophobic box consisting of PheP8 and TrpP13 from one peptide and TyrP4 and CysP15 from the other peptide. The polar interactions are located mainly at the bottom of the binding crevice and are mainly with loop L5 in D2. Five of the six hydrogen bonds are between the mainchain of the β-turn residues Gly^{P9}, Pro^{P10} and Leu^{P11} from one peptide with the mainchain and sidechain hydroxyl of conserved TyrP4, which crosses over its other peptide partner, to interact with loop L3 (Table 2). The EBP-EBP interaction makes a surprisingly minor contribution to the overall stability of the complex where the interreceptor buried molecular surface is only 75 Å², contributed by Leu¹⁷⁵ and Arg¹⁷⁸ from each receptor molecule.

EMP1 is one of a family of sequences that contain several conserved residues, besides the cysteines (**EXECUTED SECTION OF THE MOST STRUCTURAL SECTION OF T

Dimerization of EBP in Solution

To explore the interaction of EMP1 with EBP in solution we employed a [1,4-di-(2'-pyridyldithio DPDPB, reactive crosslinker bifunctionalsulphydryl propionamido) butane], in an attempt to stabilize a peptide-dependent dimeric structure. The choice of crosslinker was based on previous experiments with amine-reactive crosslinkers that were found to inactivate EBP. EBP contains a single free sulphydryl (Cys¹⁸¹) in D2 which is potentially reactive to crosslinking reagents (The DPDPB crosslinker itself does not inactivate the EPO binding potential of EBP nor the proliferative properties of EMP1). A dimeric EBP product is formed by co-incubation of EMP1, DPDPB and EBP. The amount of dimeric product increases with peptide concentration and no significant dimer product is observed in the absence of peptide. DPDPB-crosslinked products formed through disulfide-exchange reactions should be readily reversible by reduction as is seen for the covalently-linked EMP1-mediated dimer. Furthermore, we have constructed a covalently-linked dimeric form of EMP1 that demonstrates increased biological potency (Johnson et al, in preparation). The Cys¹⁸¹ residues in D2 of the EBP dimer are 20.7 Å apart (Sy-Sy distance) which approximates the 16 Å length (and approximately 2 Å in bond length at each end) of the DPDPB crosslinker. Thus EMP1 mediates formation of a soluble EBP dimer complex in solution consistent with the crystal structure.

The WSXWS motif

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The WSAWS sequence (residues 209-213) corresponding to the WSXWS box occurs in a β -bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) immediately preceding β -strand G in D2. Residues in this motif do not interact with ligand, have no role in receptor-receptor interactions and are located on the opposite side of the receptor-receptor and receptor-ligand interface. The WSAWS box represents only a segment of a complex array of interactions that involves several other conserved side chains from the four-stranded β -sheet in D2. The indole ring systems of Trp²⁰⁹ and Trp²¹² point toward an external concave surface of the β -sheet and are only partially solvent exposed, whereas the Ala²¹¹ side chain points directly out into solution. The amides and hydroxyls of both Ser²¹⁰ and Ser²¹³ form hydrogen bonds with the main

chain of residues 198 and 196 of adjacent strand F in a pseudo β -sheet type interaction that resembles a modified wide \beta-bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) where the sidechain hydroxyl rather than the carbonyl oxygen makes the β -sheet interaction. The β -bulge architecture places the two Trp residues, which are spread four residues apart, on the same side of the β-sheet and not on opposite sides as in normal β -sheet or extended chain structures. The guanidinum group of Arg¹⁹⁷ from Strand F, the central residue (Richardson, Adv. Prot. Chem. 34: 167, 1981; Chan et al., Protein Science, 2:1574, 1993) in the bulge, is positioned exactly between the two Trp indole rings to form an extended π -cation system (Kumpf et al., Science 261:1708, 1993. The center of the pyrrole ring of Trp²⁰⁹, the NE of the Arg¹⁹⁷ and the center of the benzene ring of Trp212 are positioned on a straight line with the three planes of the conjugated systems stacked parallel to each other at approximately 4 Å spacing. In addition, the aliphatic portion of the Arg¹⁹⁹ side chain has hydrophobic interactions with the indole ring of Trp209, completing the alternating stacking of two aromatic and two positively-charged amino acid residues. The side chain of Glu¹⁵⁷ forms a hydrogen bond with Arg¹⁹⁷ presumably to help orient the guanidinium group and add some specificity and stabilization to the system.

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It appears then that the linear WSXWS motif identified from sequence alignments of cytokine receptors represents only a component of a more complex conformational unit that contributes a significant structural feature to D2. Aromatic residues have previously been suggested to have a stabilizing effect and play a role as a folding nuclei in structures of antiparallel β -sandwiches (Finkelstein et al., Protein Eng. 6:367, 1993). The aminoaromatic parallel stacking between the guanidinium group of arginine and the aromatic rings is a common feature in protein structures (Burley et al., Adv. Prot. Chem., 39:125, 1988; Flocco et al., J. Mol. Biol., 235:709, 1994), but a parallel triple stacking of π -cation systems is rare (Kim et al., Biochemistry 32:8465, 1993) although observed in other class-1 cytokine receptors, hGHbp and PRLR.

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The structural equivalents of the WSXWS motif in hGHbp (YGEFS) and PRLR (WSAWS) are involved in an even more intricate and complex array of π -cation interactions. The π -cation system is extended in hGHbp and PRLR to include an additional aromatic residue (Trp186 for hGHbp and Trp156 for PRLR) from the loop region that links βC and $\beta C'$ in D2 and a positively-charged residue (Arg²¹¹ for hGHbp and Arg147 for PRLR) that stacks between the Trp and the second aromatic residue. The additional Arg residue is contributed either from the βF strand as in hGHbp (Arg²¹¹) or from BC as in PRLR (Arg147); the glutamine residue that hydrogen bonds and orients the arginine also switches strands. Sequence alignments suggest that this Arg-Gln switch could be common to other members of the class-1 cytokine receptor family. The extended π -cation system in hGHbp and PRLR consists of five positively charged and three aromatic residues stacked in an alternating order which comprises of Lys²¹⁵, Tyr²²², Arg²¹³, Phe²²⁵, Arg²¹¹, Trp¹⁸⁶, Lys¹⁷⁹ for hGHbp and Lys¹⁸⁵, Trp¹⁹¹, Arg¹⁸³, Trp¹⁹⁴, Arg¹⁴⁷, Trp¹⁵⁶, Lys¹⁴⁹ for PRLR. The first aromatic-Arg-aromatic trio are approximately 4Å apart, as in EBP, but the second system is stacked closer together at approximately 3.6 Å spacings consistent with π - π interaction (Burley et al., Adv. Prot. Chem., 39:125, 1988; Flocco et al., J. Mol. Biol., 235:709, 1994). The outer lysines also use the aliphatic portions of their side chains to form hydrophobic interactions with the aromatic rings. Based on sequence alignments with other members of the class-1 cytokine receptor superfamily, such structurally extended π -cation systems could exist in human thrombopietin, IL-6 and ciliary neurotrophic factor receptors, and in human IL-4 receptor based on structural modeling (Gustchina et al., Proteins 21:140, 1995). Although IFNγRα and tissue factor do not have a WSXWS motif, the corresponding sequences TTEKS (residues 213-217) for IFN-γRα (Walter et al., Nature 376:230, 1995) and KSTDS (residues 201-205) for tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994), maintain a very similar β-bulge. The consensus sequence among these five x-ray structures indicates that a serine or threonine in positions 2 and 5 maintain a common set of hydrogen bonds between their side chain hydroxyls and the mainchain of the neighboring strand. Only in hGHbp is there no hydroxyl-containing residue in position 2, but Ser²²⁶ still maintains the equivalent interaction. A Ser²²⁶ to Ala mutation abrogates hGHR binding to hGH, and its expression on the cell surface is drastically reduced (Baumgartner et al., J. Biol. Chem., 269: 29094, 1994). In GM-CSFR α and IL-2R β , point mutations of the serine residues cause a substantial decrease in cell surface expression but little or no effect on ligand binding (Ronco et al., J. Biol. Chem. 269:277, 1994; Miyazaki et al., EMBO Journal 10:3191, 1991).

Conservation of the WSXWS motif in EPOR or its equivalent in other members of the class 1 cytokine receptors has been proposed to be essential for biological activity and was thus assumed to be part of the receptor binding site (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle, Mol. Cell. Biol. 12:4553 1992). For EPOR, a systematic study of 100 mutations of the WSAWS sequence demonstrates that most of the mutations of the two tryptophan and serine resulted in molecules that did not reach the cell surface but were retained in the endoplasmatic reticulum (Hilton et al., Proc. Natl. Acad. Sci. USA 92:190, 1995; Hilton et al., J. Biol. Chem. 271:4699, 1996). Furthermore, an Ala²¹¹ to Glu mutation in the WSAWS sequence resulted in better transportation from the ER to the Golgi and a 3-5 fold increase of the number of EPOR molecules on the cell surface compared to the wild-type (Hilton et al., Proc. Natl. Acad. Sci. USA 92:190, 1995; Hilton et al., J. Biol. Chem. 271:4699, 1996). These results support our conclusion that the WSXWS sequence plays an important role in the structure and folding of D2 in EPOR and other related receptors.

Comparison with other cytokine-receptor complex structures

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The overall quaternary structure of the peptide-EBP complex substantially from the equivalent arrangement in the hGH-hGHR complex. The non-symmetric nature of the single four-helix-bundle structure of the growth hormone ligand results in an asymmetric homo-dimerization of the receptor that corresponds to a 159° rotation between receptors compared to the almost perfect 2-fold (180°) rotation for the EBP-peptide complex. The tertiary arrangement of domains within EBP and hGHbp is also somewhat different. When the equivalent EBP and hGHbp D2 domains are superimposed on each other, their corresponding D1 domains differ by a 12° rotation and a 4.3Å translation.

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The mechanism of hGH binding to its receptor has been well studied (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) and is sequential. Initial high affinity (nM) binding of the hormone with one receptor results is a buried surface of 1130 Å² on the receptor. The second hGHbp2 has a substantially smaller interface (deVos et al., Science 255:306, 1992) with the second binding site on hGH and interacts only with the preformed 1:1 complex to generate buried surface areas of 740 Å² with hGH and 440 Å² with the first hGHbp1 (deVos et al., Science 255:306, 1992; (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995). The binding determinants of each hGHbp are comprised of the six recognition loops (L1-L6), three of which (L1-L3) come from one end of the β-sandwich structure in D1, one from the interdomain linker and two from D2.

Although these two receptor complexes, EBP-EMP1 and hGH-hGHbp, have different dimeric arrangements, which probably in this case represent differences in the size and shape of the natural versus synthetic ligand, both receptors share equivalent ligand recognition loops, L1, L3, L5 and L6 for the EBP and L1 to L6 for the hGHbp. A nonactive PRLR, complexed with only one molecule of hGH, also uses the same contact loops (L1 to L6) (Somers et al., Nature 372:478, 1994). Based on similarity of the ligand recognition sites in hGHbp and PRLR, one would expect that the binding site of EBP, when its natural EPO ligand is bound, would extend to include two additional loops, L2 and L4, that comprise residues 59-63 (L2) between strands C to C', and residues 110-118 (L4) from the carboxyl end of βG in D1 and the interdomain linker. These six loops in EBP, hGHbp and PRLR area in structurally equivalent positions but vary in size, amino acid composition and conformation although the interacting portions of each loop (side or tip) remain similar; L1, L2, L3, L5 interact mainly with their tips and L6 with its side. In EBP, the L5 loop is three residues shorter than in hGHbp and PRLR, where the L6 loop is three and four residues longer than in hGHbp and PRLR, respectively. The L2 loop also varies (6 to 10 residues) among the three receptors but in EBP does not participate in peptide binding, and in hGHbp is partially disordered, although it does contact the hormone. In one respect, this situation is similar to the complementarity-

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determining regions (CDR's) in antibodies, where changes in length and sequence of the six binding loops impose specificity for different antigens, whereas the framework itself remains constant (Wilson et al., Ciba Foundation Symposium. Wiley, Chichester, 1991, Vol. 159, p. 13).

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It has been shown for the hGH-hGHbp complex that only a subset of 9 out of 33 interacting residues that make up the structural epitope of the receptor constitute a functional epitope or hot spot (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) where high affinity binding interaction takes place. This reduced epitope is substantially smaller than the structural epitope and is comprised from residues (Arg⁴³, Glu⁴⁴, Ile¹⁰³, Trp¹⁰⁴, Ile¹⁰⁵, Pro¹⁰⁶, Asp¹⁶⁵, and Trp¹⁶⁹) which are located in contact loops L1, L3 and L5 with the most significant contribution (>4.5 kcal/mol) coming from two aromatic residues (Trp¹⁰⁴ and Trp¹⁶⁹) in L3 and L5 (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells, Proc. Natl Acad. Sci. USA 93:1, 1996). In EBP, Phe⁹³ is equivalent to Trp¹⁰⁴ in hGHbp, as suggested previously (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells. Proc. Natl Acad. Sci. USA 93:1, 1996; Jolliffe et al., Nephrol. Dial. Trans. 10:suppl. 2, 28, 1995), but there is no homologous residue to Trp¹⁶⁹ in the shorter L5 loop. In the EBP-EMP1 complex, the PheP8 peptide aromatic side chain occupies the equivalent position of the Trp 169 side chain in hGHbp. One can assume that when EPO binds to its receptor, the hormone may provide an aromatic residue to the hydrophobic core of the binding interface and/or the L6 loop in EBP may play a more significant role in the hormone binding than in hGHbp, since it is 3 residues longer and contains the aromatic Phe²⁰⁵.

In these three class-1 receptor structures, some loops are disordered which are in D2 for EBP for EBP (residues 164-166 in EBP1 and 133-135 in EBP2) and in D1 for both hGHbp (residues 55-58, 73-78 for hGHbp1 and 54-60, 73-75 for hGHbp2) and PRLR (residues 31-33, 84-86). Otherwise, these three class-1 cytokine receptors do not differ greatly in their over all tertiary structures; D1 and D2 have broadly similar general

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arrangement in all three receptors such that the angle between the long axes of the two domains is approximately 90 degrees. I tis this arrangement of domains that allow these particular L1-L6 loops to be available for the recognition and binding of ligands. In a 2:2 complex between IFN-γ and its class-2 receptor IFN-γRα, D1 and D2 are related by a 125 degree angle, which elongates the receptor and restricts the binding determinants that can be used for interaction with hormone; the L1 loop now becomes buried in the D1-D2 interface, although the other five loops (L2-L6) are still available for ligand interaction. This elongated interdomain arrangement is also observed in tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994) which has a distant relationship to the cytokine receptor superfamily.

A mutational analysis of the EBP molecule indicates that the most crucial amino acid residue for binding EPO is Phe⁹³ in the L3 loop (Jolliffe et al., Nephrol. Dial. Trans. 10:suppl 2,28, 1995). The Phe93Ala mutant shows an increase int he IC₅₀ compared to the wild-type by a factor of approximately 1000, whereas other mutants (Ser91Ala, Ser92Ala, Val94Ala, Met150Ala and His153Ala) show small relative increases in teh IC₅₀ of only 2.5-12.5 fold). The side chain of Phe⁹³ buries 66 Å² of molecular surface, which is the highest among interacting side chains. In hGHbp, the corresponding Trp104Ala mutation results in an increase in the K₄ by a factor of more than 2,500 compared to the wild-type indicating the equivalent importance of this residue in hGH binding and its key contribution to the hydrophobic core of the functional epitope (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Bass et al. Proc. Natl. Acad. Sci. USA 88:4498, 1991).

The role of dimerization on signal transduction

In the EBP-EMP1 complex structure, we surprisingly observe that a peptide, unrelated in sequence and probably in structure, to the natural ligand, can induce a biologically active dimerization of EPO receptor that promotes signal transduction and cell proliferation. Comparison of three class-1 cytokine receptor complexes, whose structures have been determined so far, suggests that when the natural EPO hormone, which is

proposed to have a structure of a four-helix bundle (Boissel et al., J. Biol. Chem. 268:15983, 1993), induces receptor dimerization, it is more likely to resemble the hGH-hGHbp assemblage. This would suggest that more than one mode of productive extracellular dimerization is permissive for intracellular dimerization of the cytoplasmic domains with two JAK2 molecules in order to initialize the cascade of events that produces the biologically relevant signal (Ihle et al., Seminars in Immunology 5:375, 1993; Klingmuller et al., Cell 80:729, 1995). The peptide-EBP structure would then represent only one possible dimeric arrangement that promotes signal transduction.

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Mutant EPOR molecules, containing a single Arg to Cys mutation (Arg¹³⁰ in human and Arg¹²⁹ in murine), have been shown to form biologically active dimers in the absence of EPO (Yoshimura et al., J. Biol. Chem. 267:11619, 1992); Watowich et al., Proc. Natl. Acad. Sci. USA 89:2140, 1992; Watowich et al., Mol. Cell. Biol. 14:3535, 1994), suggesting that extracellular recptor homo-dimerization may be sufficient in itself for signal transduction. It has been shown in another system (Spencer et al., Science 262:1019, 1993) that activation of a specific set of transcription factors can be induced by the chemical crosslinking of cytoplasmic domains of modified cell membrane receptors that do not contain the extracellular and transmembrane domains. These receptors are not related to the cytokine receptor superfamily but illustrate that oligomerication plays a key role in activation of the receptor, and that the main functional role of the extracellular, ligand-binding domain is to allow (in the presence of ligand) dimerization or oligomerization and induce similar association of the cytoplasmic domains.

Mutageneses experiments originally suggested a role for the WSXWS motif in this cell signalling process (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle et al. Mol. Cell. Biol. 12:4553, 1992; Chiba et al., Biochem. Biophys. Res. Comm. 184:485, 1992) possibly by promoting receptor homo-dimerization. However, truncation mutants of EPOR (Miura et al., Arch. Biochem. Biophys. 306:200, 1993) do not confirm this role for the WSXWS motif. The EBP-EMP1 complex structure shows that the WSXWS motif

of the EPOR, as for the hGH-hGHbp complex (deVos et al., Science 255:306, 1992) is located on the opposite face of the molecule from the receptor dimerization. In the absence of unliganded structures for the extracellular domains of EPOR, hGHR and PRLR, it is not possible to determine whether any conformation change occurs on ligand binding that would involve the WSXWS box. Apart from being a striking structural feature in D2, and its obvious proximity to the membrane spanning domain, one cannot rule out possible interactions of this region with some other cell surface molecules that are involved somehow in the signal transduction process.

Towards design of small molecule mimetics

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The structure of the EMP1 dimer demonstrates that a peptide considerably smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide can be assumed to form a substantially smaller contact interface than the natural hormone with the receptor. The peptide binding site in EBP forms an almost flat surface, which is mainly hydrophobic in nature, without any cavities or charged residues that are normally essential for the specific targeting of small molecule ligands to a receptor binding site. The hGHbp study (Wells et al., Science 267:383, 1995; Wells, Proc. Natl. Acad. Sci. USA 93:1, 1996) shows that only a small part of the observed structural binding site, the so-called functional epitope (supra), contributes most of the binding energy and strongly implied that a "minimized" hormone designed to interact with this site could form sufficient interactions to activate the receptor. Furthermore, the limited site of interaction of the small agonist peptide with the EBP corresponds almost exactly to the smaller functional epitope derived from alanine scanning of hGH and hGHbp. Thus, by a different approach, we have arrived at the similar conclusion that a small number of key interactions can contribute to a functional epitope on a receptor. Understanding of this simplified interaction surface can be now combined with further mutational studies to assist in identifying the most crucial residues in the functional epitope, and consequently provide a more practical target for drug design.

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The crystallographic data is summarized in Table 1. Native crystallographic data were collected on a Siemens multiwire area detector mounted on an Elliott GX-18 generator, operating at 40kV and 55mA, with a crystal-to-detector distance of 120mm. Two derivative data sets were collected on a MAR image plate mounted on a Siemens generator operating at 50kV and 80mA, with crystal-to-image plate distance of 150mm. Data were integrated, scaled and reduced using the programs XENGEN (Howard et al., J. App. Cryst. 20:383, 1987) for the native data and DENZO/SCALEPACK (Otwinowski et al., SERC Darsbury Laboratory, Warrington, 1993) for the derivative data. Initial multiple isomorphous replacement anomalous scattering (MIRAS) phases were calculated to 3.1 Å using the program package PHASES (Furey, American Crystallographic Association Fortieth Anniversary Meeting, New Orleans, LA, 1990) with a mean figure of merit of 0.64 (25.0-3.1 Å). Phases were refined in PHASES using the solvent flattening protocol to a mean figure of merit of 0.92 (25.0-3.1 Å). The quality of the map was generally good and most of the complex structure (94%) could be fitted using the graphics program O (Jone et al., Acta Crystallogr A47:110, 1991). The register of the amino acid residues was verified from the positions of the two disulfide bridges in D1. and the positions of the two Hg's from the mercury acetate derivative that were correctly assumed to bind to the free Cys¹⁸¹ residue. the peptide interpretation was verified from another data set from a complex between EBP and an iodinated peptide (TyrP4 was substituted for p-iodo-Phe), which diffracted to 3.3Å resolution, that in difference Fourier (Find-Fnut) and a clear indication of the location of the iodine atoms. The structure was refined using the slow-cooling protocol in X-PLOR 3.1(Brunger et al., Acta Crystallogr A46:585, 1990; Brunger, X-PLOR, Version 3.1: A System for X-ray and NMR, Yale Univ. Press, New Haven, CT, 1992) and rebuilt using Fo-Fc, 3Fo-2Fc and SIGMAA(Read, Acta Crystallogr. A42:140, 1986) weighted electron density maps. After every two cycles of refinement, a set of simulated annealing omit maps (7-10%) to reduce model bias was calculated and the entire structure rebuilt. After several cycles of refinement, individual temperature factors were calculated and after 10 cycles of refinement and model building, the R-value was 0.21 for 8.0-2.8 Å data with F>10 (13,984 reflections). The average thermal parameters for receptor I, receptor II and the

peptides are 10.5Å², 12.3Å and 10.7Å respectively. Only one non-glycine residue [Asn¹⁶⁴ in EBP2], located in a loop region in D1, is in a disallowed region in the Ramachandran plot. No solvent molecules were included in the model due to the moderate resolution (2.8 Å) of the structure determination.

5 Binding Contacts

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Binding contacts are summarized, in part, in Table 2: Hydrogen bond interactions in the binding site of the EBP-EMP1 complex. Due to the symmetrical nature of the complex, peptide-1 and peptide-2 have equivalent interactions with the two EBP molecules. The hydrogen bond interactions were analyzed using HBPLUS (McDonald et al., J. Mol. Biol. 238:777, 1994), based upon both distance (3.9 Å cutoff) and geometrical considerations.

A number of embodiments of the present invention have been described. Nevertheless, it will be understood that various modifications may be made without departing from the spirit and scope of the invention. Accordingly, it is to be understood that the invention is not to be limited by the specific illustrated embodiment, but only by the scope of the appended claims.

all.con		•	Thu 1	pr 25	15	:08:	07 1	996	1	
EBP 1	-PE	PTI	DE1							
VDW	1 .	LEU	33	CB	4	PHE	308	CE1	1	3.95
VDW VDW		LEU	33	CB 、	4	PHE	308		1	4.11
VDW		PHE PHE	93 93	CE1	4	TRP TRP	313 313		1	3.74
VDW		PHE	93	.CZ	4	TRP	313		1 1	3.98 4.08
VDW		PRO		CA	4	GLY	309		i	3.59
VDW VDW		PRO		CB	4	GLY	309		1	3.49
VDW		PRO MET	149 150	C N	4	GLY PRO	309 310	•	1	3.66
VDW		MET	150	N	4	PRO	310	-	1 1	3.35 3.62
VDW		MET	150	CA	4	LEU	311	Ö	ì	3.41
VDW VDW		MET	150	CA	4	GLY	309	-	1	3.78
VDW	-	MET MET	150 150	CA CG	4	LEU PHE	311 308	C CD2	1	3.87
VDW		MET	150	CG	4	PHE	308	CB CB	1 1	3.50 3.70
VDW	1 1	MET	150	CG	4	PHE	308	CG	i	3.79
VDW		MET	150	SD	4	PHE	308	CD2	1	3.52
VDW VDW		MET MET	150 150	SD SD	4	THR	312	С	1	3.55
VDW		MET	150	SD	4	THR	312 313	CA N	1	3.58
VDW		MET	150	SD	4	PHE	308	CA	1 1	3.75 3.91
VDW		MET	150	SD	4	PHE	308	CB	î	4.03
VDW		MET	150	CE	4	PHE	308	CD2	1	3.45
VDW VDW		MET MET	150 150	CE CE	4	TRP PHE	313 308	CE2	1	3.71
VDW		MET	150	CE	4	TRP	313	CE2 CD2	1 1	3.79 3.83
VDW	1 1	MET	150	CE	4	TRP	313	NE1	1	3.91
VDW		MET	150	CE	4	TRP	313	CZ2	ī	4.10
VDW VDW		MET	150	C	4	LEU	311	0	1	3.41
VDW			151 151	N CA	4	LEU PRO	311 310	0	1	3.45
VDW			151	CB	4		310	0	1 1	3. 82 3.56
VDW	1 2		151	OG1	4	LEU	311	CD2	i	3.43
VDW			151	OG1	4	LEU	311	CA	ī	3.91
VDW VDW			151	CG2	4	PRO	310	0	1	3.60
VDW		HIS	152 153	CB ND1	4	LEU	311 311	0	1	3.54
SHORTVDW		HIS	153	CEl	4	THR	312	OG1	1 1	3.57 2.87
VDW		RIS	153	CE1	4	THR	312	CB	ī	3.48
VDW		ZIE	153	CE1	4		312	CA	1	3.76
VDW VDW		HIS	153 205	NE2 CE2	4	THR PHE	312	OG1	1	3.57
VDW			205	CZ	4	PHE	308	CZ CE2	1	3.90 3.40
VDW			205	CZ	4	PHE	308	CZ	î	3.53
VDW E	BP2-			C3		m	2.2			
VDW VDW			591 591	CA CB	4	TYR TYR		OH	1	3.44
VDW			591	CB		PRO		OH CB	1	3.88
VDW .	2 5	SER	591	OG	4	TYR		OH	1	3.95 3.44
VDW	2 5		591	OG	4	PRO		CB	1	3.61
VDW VDW		SER SER	591	OG OG	4	TYR		CZ	1	3.83
VDW			591	OG C	4 4	TYR TYR		CE2	1	3.84
VDW	2 \$		592	N	4	TYR		OH CE2	1	3.62 3.66
VDW	2 5	SER	592	N	4	TYR	304	CZ	1	3.68
VDW			592	CA	4	TYR	304	OH	1	3.80
VDW VDW			592 592	CB	4	TYR		ОН	1	3.73
VDW			592	C 0	4 4	TYR TYR		CE2 CE2	1	4.00
VDW	2 \$		592	Ö	4	PRO		CD	1	3.53 3.59
VDW		PHE	593	СВ	4	CYS		0	i	3.74
VDW VDW		PHE	593	CD1	4	CYS	315	CB	1	3.55
¥ D#	2 1	nL	593	CD1	4	TYR	304	CD2	1	3.72

all.com	Thu Apr 25 1	5:08:07 1996	2
VDW	2 PHE 593 CD1 2 PHE 593 CE1 2 VAL 594 CG1	4 TYR 304 CE2 4 CYS 315 CB 4 PRO 317 CG	1 3.90 1 3.71 1 3.17
SHORTVDW	2 VAL 594 CG1	4 PRO 317 CD	1 3.23
EBP1	-PEPTIDE2 1 SER 91 CB	4 PRO 417 CB	1 3.84
VDW VDW	1 SER 91 .CB 1 SER 91 CB	4 PRO 417 CG	1 3.90
VDW	1 SER 91 OG	4 PRO 417 CB	1 3.90 1 3.82
VDW	1 SER 92 N	4 TYR 404 CE2 4 TYR 404 OH	1 3.85
VDW	1 SER 92 CA 1 SER 92 CB	4 TYR 404 OH 4 TYR 404 OH	1 3.42
VDW VDW	1 SER 92 CB 1 SER 92 CB	4 TYR 404 CZ	1 4.04
VDW	1 SER 92 CB	4 TYR 404 CE2	1 4.09 1 3.43
VDW	1 PHE 93 CB	4 CYS 415 O 4 TYR 404 CE2	1 3.43
VDW	1 PHE 93 CD1	4 TYR 404 CE2 4 TYR 404 CD2	1 3.83
VDW	1 PHE 93 CD1 1 PHE 93 CD1	4 CYS 415 CB	1 3.92
ADM ADM	1 PHE 93 CE1	4 CYS 415 CB	1 4.08
VDW	1 PHE 93 CE1	4 TYR 404 CE2	1 4.09 1 3.54
VDW	1 VAL 94 CG1	4 PRO 417 CG 4 PRO 417 CD	1 3.54
VDW	1 VAL 94 CG1 1 VAL 94 CG2	4 PRO 417 CG	1 4.11
VDW EBP2	-PEPTIDE2		. 214
SHORTVDW	2 LEU 533 CB	4 PHE 408 CE1	1 3.14 1 3.77
VDW	2 LEU 533 CB 2 LEU 533 CB	4 PHE 408 CD1 4 PHE 408 CZ	1 4.00
VDW	2 LEU 533 CB 2 LEU 533 CG	4 PHE 408 CE1	1 4.05
VDW VDW	2 LEU 533 CD1	4 PHE 408 CE1	1 3.75
VDW	2 LEU 533 CD1	4 PHE 408 CZ	1 3.92 1 3.67
VDW	2 LEU 533 O	4 PHE 408 CE1 4 TRP 413 CH2	1 3.34
VDW	2 PHE 593 CE1 2 PHE 593 CE1	4 TRP 413 CZ2	1 3.41
VDW VDW	2 PHE 593 CZ	4 TRP 413 CZ2	1 3.67
VDW	2 PHE 593 CZ	4 TRP 413 CH2	1 3.96 1 3.79
VDW	2 PRO 649 CA	4 GLY 409 O 4 GLY 409 O	1 3.56
VDW	2 PRO 649 CB 2 PRO 649 C	4 PRO 410 O	1 3.72
VDW VDW	2 MET 650 CA	4 PRO 410 O	1 3.59
VDW	2 MET 650 CA	4 GLY 409 O	1 3.67 1 3.77
VDW	2 MET 650 CA	4 LEU 411 O 4 PHE 408 CD2	1 3.80
VDW	2 MET 650 CG 2 MET 650 CG	4 PHE 408 CG	1 3.92
VDW VDW	2 MET 650 CG 2 MET 650 CG	4 PHE 408 CB	1 4.05
VDW	2 MET 650 SD	4 TRP 413 N	1 3.72 1 3.75
VDW	2 MET 650 SD	4 THR 412 C 4 PHE 408 CD2	1 3.75 1 3.76
VDW	2 MET 650 SD .2 MET 650 SD	4 THR 412 CA	1 3.78
VDW VDW	2 MET 650 SD	4 PHE 408 CA	1 4.02
VDW	2 MET 650 CE	4 TRP 413 CE2	1 3.67 1 3.76
VDW	2 MET 650 CE	4 TRP 413 NE1 4 TRP 413 CD2	1 3.76
VDW	2 MET 650 CE 2 MET 650 CE	4 PHE 408 CD2	1 3.83
VDW VDW	2 MET 650 CE	4 TRP 413 CD1	1 3.88
VDW	2 MET 650 CE	4 TRP 413 N	1 3.89
VDW	2 MET 650 CE	4 TRP 413 CG 4 LEU 411 O	1 3.90 1 3.54
VDW	2 MET 650 C 2 MET 650 C	4 LEU 411 0 4 PRO 410 0	1 3.57
VDW VDW	2 MET 650 C 2 THR 651 N	4 LEU 411 0	1 3.56
VDW VDW	2 THR 651 N	4 PRO 410 C	1 3.77
VDW	2 THR 651 CA		1 3.41 1 3.03
SHORTVI	OW 2 THR 651 CB		1 3.98
VDW VDW	2 THR 651 CB 2 THR 651 CB		1 4.02
VDW VDW	2 THR 651 OG		1 3.62

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VDW	2	SER	652	N	4	LEU	411	С	1	3.83	
VDW	2	SER	652	CA	4	LEU	411	Ö	ī	3.51	
VDW	2	SER	652	CB	4	LEU	411	Ö	ī	3.18	
VDW	2	SER	652	CB	4	LEU	411	Č	ī	4.09	
VDW	2	SER	652	oe.	4	THR	412	CB	ī	3.73	
SHORTVDW	2	HIS	653	.CE1	4	THR	412	OG1	1	3.00	
VDW	2	HIS	653	CE1	4	THR	412	CB	1	3.91	
PEPTIDE1-PEPTIDE2											
SHORTVDW	3	THR	303	OG1	4	HIS	407	CB	1	2.94	
VDW	3	THR	303	OG1	4	HIS	407	CA	1	3.61	
VDW	3	TYR	304	CB	4	CYS	406	0	1	3.86	
VDW	3	TYR	304	CD1	4	TRP	413	CZ3	1	3.81	
VDW	3	TYR	304	CD1	4	TRP	413	CH2	1	3.94	
VDW	3	TYR	304	0	4	CYS	406	N	1	3.33	
VDW	3	TYR	304	0	4	CYS	406	0	1	3.47	
VDW	3	TYR	304	0	4	SER	405	CA	1	3.57	
VDW	3	SER	305	CA	4	TYR	404	0	1	3.51	
VDW	3	SER	305	С	4	TYR	404	0	1	3.77	
VDW	3	CYS	306	0	4	THR	403	CB	1	3.50	
VDW	3	CYS	306	0	4	TYR	404	CB	1	3.54	
VDW	3	CYS	306	0	4	TYR	404	CD1	1	3.59	
VDW	3	CYS	306	0	4	TYR	404	CA	1	3.75	
VDW	3	CYS	306	CB	4	CYS	406	SG	1	3.81	
VDW	3	CYS	306	SG	4	CYS	406	SG	1	3.75	
VDW	3	CYS	306	SG	4	CYS	406	CB	1	4.06	
VDW	3	PHE	308	CEl	4	TYR		OH	1	3.93	
VDW VDW	3	PHE	308	CE1	4	TYR	404	CE1	1	4.08	
	3	TRP	313	CG	4	TRP	413	CD1	1	3.85	
SHORTVDW VDW	3	TRP	313	CD1	4	TRP	413	CD1	1	3.04	
ADM ADM	3	TRP	313	CD1	4	TRP	413	NE1	1	3.37	
VDW VDW	3	TRP	313	CD1	4	TRP	413	CG	1	4.09	
VDW	3 3	TRP	313 313	NE1	4	TRP	413	CD1	1	3.31	
ADM ADM	3			CZ2	-	CYS	415	SG	1	3.84	
VDW VDW	3	TRP	313 315	CH2	4	CYS	415	SG	ı	3.83	
VDW VDW	3 3	CYS	315	SG	4	TRP	413	CZ2	1	3.59	
VDW	<i>3</i>	CYS	315	SG	4		413	CE2	1	3.95	
VDW	3		318	SG CD	4	TRP	413 418	CH2	1	4.00	
VDW	3		318	OE1	4	SER		NE2	1	3.28	
V DN	3	GUN	310	UEL	4	SER	405	CB	1	3.80	

bref2lc.pdb Thu Apr 25 12:27:47 1996

THE COMPLEX BETWEEN THE EXTRACELLULAR DOMAIN OF ERYTHROPOIETIS REMARK REMARK RECEPTOR (EBP) AND AN AGONIST EPO MIMETIC PEPTIDE 1 (EMF1) REMARK ***** WARNING **** RESIDUES 21-23 (521-523) and 164-166, 633-636 REMARK HAVE WEAK OP. NO ELECTRON DENSITY MAP AND HAVE BEEN MODELED INTO THE STRUCTURE. THESE RESIDUES HAVE A HIGH B OF 90. REMARK REMARK THE STRUCTURE CONSISTS OF TWO RECEPTOR (RESIDUES 10-220, 510-720) REMARK AND PEPTIDE (RESIDUES 303-318, 403 418) MOLECULES. REMARK 1.00 22.57 40.090 29.257 22.042 LYS 10 1 N MOTA 1.00 23.45 39.634 30.133 20.962 10 MOTA 2 CA LYS 38.753 29.361 19.979 1.00 22.87 CB LYS 10 MOTA 3 18.735 1.00 22.92 38.334 30.155 ATOM 4 CG LYS 10 29.212 17.552 1.00 24.27 38.119 CD LYS 10 ATOM 17.890 1.00 26.55 37.165 28.015 10 6 CE LYS ATOM 17.998 1.00 26.18 35.685 28.367 LYS 10 NZ ATOM 21.420 1.00 22.91 38.921 31.427 10 ATOM 8 С LYS 39.589 32.442 21.636 1.00 24.17 Q 0 LYS 10 MOTA 31.386 21.640 1.00 21.40 37.602 MOTA 10 N PHE 11 36.868 32.588 22.026 1.00 13.56 AD PHE 11 MOTA 11 32.257 22.725 1.00 19.07 35.549 CB PHE 11 ATOM 12 34.497 33.362 22.609 1.00 20.24 CG PHE 11 MOTA 13 34.862 34.717 22.670 1.00 19.49 CD1 PHE 11 ATOM 14 33.142 33.038 22.400 1.00 19.51 CD2 PHE 11 MOTA 22.527 1.00 19.64 35.728 CE1 PHE 33.910 11 1 € ATOM 22.257 1.00 20.10 CE2 PHE 11 32.180 34.041 17 ATOM ..00 19.48 ..00 19.32 35.395 22.321 CZ. PHE 32.568 11 18 MOTA 33.567 22.887 PHE 11 37.644 С 19 ATOM 34.740 22.516 1.00 18.89 37.77€ PHE 11 0 ATOM 20 1.00 20.71 38.181 33.106 24.016 GLU 12 MOTA 21 N Ē 38.905 34.036 24.886 1.00 20.59 GLU 12 MOTA 22 CA 39.253 33.423 26.246 1.00 21.48 GLU 12 ATOM 23 CB 34.309 27.123 1.00 23.60 40.185 12 MOTA 24 CG GLU 39.455 35.301 28.056 1.00 25.09 CD GLU 12 MOTA 25 40.024 36.417 28.275 1.00 23.07 OE1 GLU 12 ATOM 26 34.952 28.589 1.00 21.05 34.539 24.172 1.00 19.22 38.356 ATOM OE2 GLU 12 28 С GLU 12 40.137 ATOM 35.703 24.334 33.687 23.341 1.00 18.49 GLU 40.513 12 29 0 ATOM 40.730 1.00 17.67 13 N SER MOTA 30 41.903 34.094 22.571 1.00 16.71 CA SEF. 13 MOTA 31 42.522 32.898 21.851 1.00 18.51 ÷. 13 ATOM 32 CB SER 32.959 20.459 1.00 23.19 42.256 33 OG SEE 13 ATOM 41.570 35.202 21.554 1.00 15.57 34 С SER 13 MOTA 1.00 15.13 21.546 42.239 36.248 ATOM 35 0 SEF. 13 40.563 34.355 20.698 1.00 12.00 N LYS 14 ATOM 36 40.117 35.912 19.675 1.00 8.51 37 CA LYS 14 ATOM 18.769 1.00 5.06 39.063 35.287 CB LYS 14 ATOM 38 34.366 17.714 39.629 1.00 2.36 ATOM 39 CG LYE 14 33.862 15.761 1.00 2.00 LYS 38.566 MOTA 40 CD 14 15.496 2.27 33.270 00. LYS 14 39,191 41 CE. ATOM 32.742 14.528 1.00 2.00 NZ LYS 14 38.193 42 ATOM 39.586 37.198 20.295 1.00 9.05 LYS 14 MOTA 43 С 39.782 38.290 19.755 1.00 7.15 LYS 14 MOTA 44 0 38.920 37.053 21.442 1.00 11.98 15 45 N ALA ATOM 22.194 1.00 12.13 1.5 38.375 38.188 46 CA ALA ATOM 23.378 37.571 37.697 1.00 11.49 CB ALA 15 ATOM 47 39.592 38.960 22.666 1.00 12.49 ALA 15 MOTA 48 40.189 22.535 1.00 13.58 39.683 ALA 15 MOTA 49 38.207 23.167 1.00 13.97 40.560 MOTA 50 . N ALA 16 41.792 38.796 23.615 1.00 14.97 CA ALA 16 51 ATOM 42.771 24.052 16 37.710 _.00 14.76 52 CB ALA. ATOM 42.361 39.567 22.426 1.00 15.45 ALA 53 MOTA 42.624 40.759 22.537 1.00 15.35 ALA 16 54 0 ATOM 1.00 16.12 42.444 38.896 21.274 ATOM 5.5 N LEU 17 43.007 39.467 20.042 1.00 15.92 56 CA LEU ATOM 38.428 13.910 43.013 1.00 15.72 LEU 5.7 CB ATOM 1" 1" 1" 44.204 37.485 13.662 2.00 17.46 LEU MOTA 58 ÇG 45.474 38.294 18.506 1.00 15.45 CD1 LEU ATOM 59 44.360 36.462 19.774 1.00 16.32 CD2 LEU MOTA 60 17 1.00 15.04 42.374 40.741 19.512 LEU ATOM 61 C 41.438 42.985 18.711 1.00 15.91 ATOM 0 LET 19.908 41.136 41.018 1.00 17.34 MOTA 63 N LEU 18 19.443 18 40.434 42,210 .00 15.72 ATOM CA LEU 38.999 41.867 19.022 1.00 13.72 ATOM 65 CB LEU 18 1.00 9.76 1.00 5.61 38.725 41.263 17.640 CG LEU MOTA 66 CD1 LEU 18 37.235 41.260 17.329 ATOM 57 ...00 10.13 42.117 16.625 CD2 LEC 18 39.422 MOTA óà LEU 20.500 C 18 40.393 43.284 .00 17.38 MOTA 69 LEU 39.876 44.375 20.257 O 18 ATOM 70

bref21	c.pc	Ъ		Thu	Apr 25 12	2:27:47	1996	2	
ATOM	71	N	ALA	19	40.921	42.981	21.680	1.00 19.88	7
MOTA	72	CA	ALA	19	40.925	43.941	22.789	1.00 22.64	ક
ATOM	73	CB	ALA	19	41.560	43.331	24.041	1.00 22.75	6
ATOM	74	С	ALA	19	41.601	45.273	22.445	1.00 25.13	ર્ક
ATOM	75	0	ALA	19	42.026	45.499	21.294	1.00 25.03	3
MOTA	76	N	ALA	20	41.649	46.164	23.453	1.00 28.77	?
ATOM	77	CA	ALA	20	42.246	47.514	23.333	1.00 28.51	6
ATOM	78	СВ	ALA	20	41.529	48.505	24.310	1.00 28.93	6
ATOM	79	С	ALA	20	43.770	47.526	23.562	1.00 27.54	6
ATOM	80	0	ALA	20	44.438	46.484	23.505	1.00 27.85	8
ATOM	81	N	ARG	2:	44.326	48.699	23.848	1.00 90.00	7
ATOM	82	CA	ARG	21	45.765	48.784	24.075	1.00 90.00	5
ATOM	83	CB	ARG	21	46.562	48.353	22.819	1.00 90.00	6
ATOM	84 85	CG CD	ARG	21 21	45.827	48.428	21.446	1.00 90.00	5
ATOM ATOM	86	NE	ARG ARG	21	45.719 44.765	49.838	20.863	1.00 90.00	6
ATOM	87	CZ	ARG	21	43.448	50.675	21.591	1.00 90.00	7
ATOM	88		ARG	21	42.915	50.471 49.448	21.610	1.00 90.00	6 7
ATOM	89		ARG	21	42.669	51.270	20.926 22.350	1.00 90.00	7
ATOM	90	С	ARG	21	46.298	50.118	24.590		5
ATOM	91	Ö	ARG	21	45.875	51.199	24.132	1.00 90.00	
ATOM	92	Ŋ	GLY	22	47.158			1.00 90.00	3 7
ATOM	93	CA	GLY	22	47.138	50.016 51.171	25.614 26.193	1.00 90.00	, 5
ATOM	94	C	GL Y	22	49.053	51.371	25.314	1.00 90.00	ó
ATOM	95	Ö	GLY	22	48.939	51.174			
ATOM	96	Ŋ	PRO	23	50.230	51.765	24.089 25.872	1.00 90.00	3 7
ATOM	97	CD	PRO	23	50.318	52.564	27.119	1.00 90.00	, 5
ATOM	98	CA	PRO	23	51.451	51.971	25.062	1.00 90.00	o 6
ATOM	99	СВ	PP.O	23	51.713	53.452	25.287	1.00 90.00	5
ATOM	100	CG	PRO	23	51.527	53.517	26.850	1.00 90.00	5
ATOM	101	С	PRO	23	52.681	51.167	25.544	1.00 90.00	ě
ATOM	102	0	PRO	23	52.560	50.067	26.123	1.00 90.00	š
ATOM	103	N	GLU	24	53.863	51.758	25.368	1.00 28.27	7
MOTA	104	CA	GLU	24	55.136	51.178	25.741	1.00 24.32	6
ATOM	105	CB	GLU	24	56.332	52.009	25.238	1.00 24.01	6
ATOM	106	CG	GLU	24	56.479	52.149	23.723	1.00 25.03	6
ATOM	107	CD	GLU	24	56.710	50.822	22.959	1.00 24.22	6
ATOM	108	OE1	GLU	24	57.171	50.954	21.793	1.00 23.14	S
ATOM	109	OE 2	GLU	24	56.430	49.692	23.478	1.00 18.50	3
ATOM	110	С	GLU	24	55.117	51.264	27.268	1.00 23.39	6
ATOM	111	0	GLU	24	54.874	52.365	27.829	1.00 24.36	3
ATOM	112	N	GLU	25	55.342	50.124	27.925	1.00 18.35	7
ATOM	113	CA	GLU	25	55.371	50.058	29.377	1.00 14.09	5
ATOM	114	CB	GLU	25	53.962	49.818	29.907	1.00 17.09	5
ATOM	115	CG	GLU	25	53.789	49.985	31.410	1.00 22.21	5
ATOM	116	CD	GLU	25	53.199	51.348	31.799	1.00 27.17	5
MOTA	117	OE1		25	53.461	52.355	31.057	1.00 27.15	5
ATOM	118		GLU	25	52.461	51.401	32.837	1.00 26.11	3
ATOM	119	Ç	GLU	25	56.249	48.872	29.725	1.00 11.99	÷
ATOM	120	0	GLU	25	56.056	47.779	29.181	1.00 14.38	3
ATOM	121	N	LEU	26	57.246	49.098	30.572	1.00 8.48	-
ATOM	122	CA	LEU	26	58.147	48.034	31.001	1.00 5.93	5
ATOM ATOM	123		LEU LEU	26	59.398	48.624	31.652	1.00 4.03	÷
ATOM	124 125	CG	LEU	26 26	60.719 61.537	47.880 48.145	31. 4 88 32.704	1.00 2.00 1.00 4.41	5
ATOM	125		LEU	26	60.535	46.401	31.317	1.00 4.41	6 6
ATOM	127	c	LEU	26	57.409	47.188	32.030	1.00 2.00	5
ATOM	128	. 0	LEU	26	56.951	47.727	33.041	1.00 9.43	3
ATOM	129	N	LEU	27	57.31C	45.880	21.797	1.00 5.17	7
ATOM	130	CA	LEU	27	56.613	44.996	32.719	1.00 5.71	Ę
ATOM	131	CB	LEU	2	55.428	44.334	32.035	1.00 5.71	ě
ATOM	132	CG	LEU	2 -	54.281	45.263	21.673	1.00 10.34	•
ATOM	133		LEU	2~	53.101	44.423	31.125	1.00 10.81	:
ATOM	134		LEU	27	53.871	46.130	32.906	1.00 7.08	÷
ATOM	135	5	LE	27	57.454	43.923	33.397	1.00 7.41	•
ATOM	136	ō	LEU	2 7	58.003	43.037	32.742	1.00 7.62	3
ATOM	137	N	TYS	28	57.460	43.964	34.726	1.00 7.42	•
ATOM	138	CA	CYS	28	58.208	43.027	35.554	1.00 4.67	
ATOM	139	C	CYS	28	57.246	42.359	36.529	1.00 4.38	÷
ATOM	140	0	CYS	28	56.217	42.945	35.861	1.00 2.56	;
MOTA	141	CB	CZ3	28	59.266	43.791	36.357	1.00 3.64	•
MOTA	142	SG	CYS	28	60.429	44.763	35.358	00 4.37	16
ATOM	143	14	PHE	23	57.599	41.153	36.977	1.00 2.00	•
ATOM	144	CA	PHE	29	56.817	40.403	37.943	1.00 2.00	45
ATOM	145	CB	PHE	29	55.474	39.899	37.322	1.00 4.36	÷
ATOM	146	CG	PHE	29	55.586	38.643	36.437	1.00 3.43	-5
MOTA MOTA	147		1 PHE	29	55.493	37.369	35.990	.00 2.00	-5
A OF	148	-D	2 PHE	29	55.790	38.747	25.058	1.00 2.00	-5

bref21	c.pdb	Thu Ap	r 25 12	:27:47	1996	3
ATOM	149 CE1 PHE	29	55.605	36.243		.00 2.00 6
ATOM	150 CE2 PHE	29	55.906	37.616		.00 2.00 5
ATOM	151 CZ PHE	29	55.815	36.365		00 2.00 6 00 3.80 f
ATOM	152 C PHE	29	57.678	39.260 38.897		1.00 2.00 5
ATOM	153 O PHE	29 30	58.702 57.340	38.814		2.00 4.17 7
MOTA	154 N THR 155 CA THP	30	58.021	37.694		i.00 3.12 é
MOTA	155 CA THR 156 CB THE	30.	58.720	38.116	41.820	1.00 2.00 6
ATOM ATOM	157 OG1 THR	30	59.337	36.982		1.00 2.00
ATOM	158 CG2 THP.	30	57.763	36.661		1.00 2.00 5
ATOM	159 C THR	30	56.951	36.601		1.00 6.81 6 1.00 8.70 3
ATOM	160 O THR	30	55.774	36.924 35.326		1.00 7.95 7
MOTA	161 N GLU	31	57.342 56.378	34.219		1.00 8.18 5
MOTA	162 CA GLU 163 CB GLU	31 31	56.577	33.240		1.00 7.89 న
ATOM ATOM	163 CB GLU 164 CG GLU	31	56.490	33.821		1.00 8.99 6
ATOM	165 CD GLU	31	56.651	32.750	37.248	1.00 10.58 6
ATOM	166 OE1 GLU	31	57.538	32.875	36.395	1.00 13.03 3 1.00 14.01 3
ATOM	167 OE2 GLU	31	55.916	31.753 33.432	37.302 42.079	1.00 8.38 6
ATOM	168 C GLU	31 31	56.453 55.437	32.940	42.582	1.00 9.78 €
ATOM	169 O GLU 170 N ARG	32	57.678	33.064	42.416	1.00 7.19 7
ATOM ATOM	171 CA ARG	32	58.006	32.390	43.670	1.00 8.64 5
ATOM	172 CB ARG	32	58.844	31.154	43.405	1.00 9.16 6
MOTA	173 CG ARG	32	58.284	30.364	42.261	1.00 10.75 6 1.00 11.21 6
ATOM	174 CD ARG	32	58.376	28.894	42.469	1.00 11.21 5 1.00 13.52 7
MOTA	175 NE ARG	32	57.070	28.271	42.295 41.187	1.00 16.55 6
MOTA	176 CZ ARG	32	56.328 56.763	28.350 29.036	40.128	1.00 17.12 7
MOTA	177 NH1 ARG 178 NH2 ARG	32 32	55.145	27.734	41.128	1.00 17.67 7
MOTA MOTA	178 NH2 ARG 179 C ARG	32	58.834	33.536		1.00 9.21 6
MOTA	180 0 ARG	32	59.004	34.526		1.00 13.37 8
ATOM	181 N LEU	33	59.382	33.499		1.00 7.72 7 1.00 8.01 5
MOTA	182 CA LEU	33	60.084	34.736		1.00 8.01 5 1.00 7.85 6
MOTA	183 CB LEU	33	59.536	35.403 36.310		1.00- 2.00 6
ATOM	184 CG LEU	33	58.323 57.061	35.584		1.00 3.91 6
ATOM	185 CD1 LEU 186 CD2 LEU	33 33	58.381	37.604		1.00 2.00 6
ATOM	186 CD2 LEU 187 C LEU	33	61.610	34.893		1.00 8.52 €
atom atom	188 0 LEU	33	62.269	35.702	46.168	1.00 10.67 8
ATOM	189 N GLU	34	62.130			1.00 6.25 7
ATOM	190 CA GLU	34	63.539			1.00 8.09 5 1.00 10.89 5
ATOM	191 CB GLU	34	64.315			1.00 18.21 6
ATOM	192 CG GLU 193 CD GLU		63.518 62.754			1.00 21.61 6
ATOM ATOM	193 CD GLU 194 OE1 GLU		61.810			1.00 22.26 €
ATOM	195 OE2 GLU		63.082	30.64		1.00 22.29 5
ATOM	196 C GL		63.678			1.00 7.89 6
ATOM	197 O GLT		64.413			1.00 10.91 3 1.00 6.40 7
MOTA	198 N ASI		62.978			1.00 4.88 5
ATOM	199 CA ASI		62.981 62.21			
MOTA MOTA	200 CB ASI 201 CG ASI		60.67			1.00 6.69 6
ATOM	202 OD1 AS		60.05			1.00 6.86 3
ATOM	203 OD2 AS		60.10			
MOTA	204 C A5		62.33			
ATOM	205 0 AS		61.56 62.67			
ATOM	206 'N LE 207 CA LE		62.09			
MOTA MOTA	208 CB LE		62.90			
ATOM	209 CG LE		62.21			2.40
ATOM	210 CD1 LE		60.99			
MOTA	211 CD2 LE		63.18			
MOTA			62.11 63.07			
ATOM			61.03			
ATOM			60.96			
MOTA MOTA			59.86			8 1.00 2.00 8
MOTA		.L 37	60.00	37.3	37 32.69	
ATOM	213 CG2 V	L 37	59.9			
ATOM			60.5			
ATOM			59.73			
ATOM		25 38 25 38	61.2 60.8			
ATOM ATOM		25 38	60.7			4 1.00 5.14 6
ATOM		YS 38	61.5		.43 30.71	.5 1.00 B.41 ⊰
ATOM	1 225 CB C	YS 38	61.8			3 1.00 2.98 6
ATOM	1 226 SG C	YS 38	61.8	60 43.3	383 34.97	2 1.00 3.22 16

bref2	lc.p	dlb		Thu	Apr 25	12:27:47	7 1996	4	
ATOM	227	N	PHE	39	59.811	42.540	30.742	1.00 4.3	5 7
ATOM	228	CA	PHE		59.621	42.507	29.286	1.00 5.38	
ATOM	229	CB	PHE	39	58.865		28. 9 00	1.00 4.80	
ATOM ATOM	230 231	CG	PHE	39 39	57.461		29.411	1.00 7.0	
ATOM	232		PHE	39	56.416 57.190		29.636	1.00 8.6	
ATOM	233		PHE		55.123		30.709 29.153	1.00 7.9	
ATOM	234		PHE	39	55.896		31.228	1.00 9.41	
ATOM	235	CZ	PHE	39	54.868		30.451	1.00 3.3	
MOTA	236	С	PHE	39	58.826		23.794	1.00 3.7	
ATOM	237	0	PHE	39	58.262		29.580	1.00 4.29	
ATOM ATOM	238 239	N CA	TRP	40 40	58.837 58.084		27.490	1.00 3.45	7
ATOM	240	CB	TRP	40	58.826		26.846	1.00 4.73	
ATOM	241	CG	TRP	40	60.014	– – –	26.872 25.928	1.00 4.45	
ATOM	242		TRP	40	61.386		26.200	1.00 7.44	
ATOM	243		TRP	40	62.143		25.062	1.00 6.04	
ATOM ATOM	244		TRP	40	62.049		27.294	1.00 10.26	
ATOM	245 246		TRF	40 40	60.003		24.661	1.00 8.12	
ATOM	247		TRP	40	61.277 63.527		24.144	1.00 6.99	
MOTA	24B		TRP	40	63.431		24.989 27.217	1.00 10.83	
ATOM	249		TRP	40	64.152		26.068	1.00 10.61	. 5
ATOM	250	С	TRP	40	57. 7 85	44.538	25.418	1.00 11.43	
ATOM	251	0	TRP	40	58.530		24.824	1.00 4.51	
ATOM	252	N	GLU	41	56.625		24.914	1.00 7.38	-
ATOM ATOM	253 254	CA CB	GLU	41 41	56.267		23.556	1.00 8.54	
ATOM	255	CG	GLU	41	5 4.89 8 54.860		23.555	7.91	
ATOM	256	CD	GLU	41	53.619		24.450 24.254	1.00 11.77	
ATOM	257	OE1	GLU	41	53.418		25.055	1.00 13.67	
ATOM	258	OE2	GLU	41	52.843	41.891	23.301	00 17.90	
ATOM	259	C	GLU	41	56.335		22.558	1.00 9.08	
ATOM	260	0	GLU	41	56.456		22.956	1.00 8.71	
ATOM ATOM	261 262	N AD	GLU	42	56.403		21.271	1.00 8.40	
ATOM	263	CB	GLU GLU	42 42	56.426 57.729		20.211	1.00 9.84	
ATOM	264	CG	GLU	42	58.974		20.227	1.00 6.56	
ATOM	265	CD	GLU	42	60.242	47.114	20.115	1.00 5.93	
ATOM	266	OE1		42	61.019		19.371	1.00 9.43	
ATOM	267	OE2		42	60.470		20.519	1.00 6.13	
ATOM ATOM	268 269	C	GLU	42	56.167		18.853	1.00 9.90	
ATOM	270	о И	GLU ALA	42 43	55.880 56.243		18.795	1.00 9.59	
ATOM	271	CA	ALA	43	55.988	46.514 46.007	17.771 16.400	1.00 10.98	
ATOM	272	CB	ALA	43	55.513	47.145	15.515	1.00 12.17	
ATOM	273	С	ALA	43	57.164	45.291	15.731	1.00 10.73	
ATOM	274	0	ALA	43	58.309	45.583	15.930	1.00 13.41	ė
MOTA MOTA	275 276	И	ALA	44	56.878	44.282	14.903	1.00 9.23	
MOTA	277	CA CB	ALA	44 44	57.928	43.514	14.208	1.00 3.02	
ATOM	278	C	ALA	44	57.326 58.828	42.507	13.263	1.00 4.97	
ATOM	279	ō	ALA	44	58.407	44.442 45.534	13.438	1.00 8.50	
ATOM	280	N	SER	45	60.086		13.275	1.00 9.5T	
MOTA	281	CA	SER	45	60.962		12.508	1.00 10.33	
ATOM	282	СB	SER	45	61.616		13.354	1.00 11.34	
ATOM ATOM	283	OG	SER	45	61.479		12.695	1.00 10.05	3
ATOM	284 · 285	0	SER SEF	45 45	61.996 62.599		11.683	1.00 13.53	÷
ATOM	286	N	ALA	46	62.113	44.571	12.124	1.00 15.72	3
MOTA	287	CA	ALA	46	63.041	44.134	9.469	1.00 14.33	
ATOM	288	CB	ALA	46	52.810	44.781	8.127	1.00 17.01	
ATOM	289	Ċ	ALA	46	64.379	44.538	19.028	1.00 15.43	
ATOM ATOM	290	5	ALA	46	64.657	45.746	10.203	1.00 16.57	3
ATOM	291 292	N CA	GLY GLY	47 47	55.140		10.433	1.00 15.71	
ATOM	293	C	GLY	47	66.450 66.558	43.762	11.009	1.00 15.77	5 5
ATOM	294	Ö	GLY	47	67.231	44.415 45.457	12.400 12.546	1.00 15.13	•
ATOM	295	N	VAL	48	65.873	43.843	13.399	1.00 16.53	÷ ;
ATOM	296	CA	VAI	48	65.950		14.799	1.00 10.23	
ATOM	297	CF	VAL	4.8	64.825	45.230	15.231	00 3.24	
ATOM ATOM	298	CG1		48	64.572	45.071	16.701	1.00 8.08	5
ATOM	299 300	CG2	VAL	48 48	65.216		14.964	1.00 6.13	
ATOM	301	õ	VAL	48	65.904 65.062		15.642	00 3.65	
ATOM	302	N	GLY	49	56.882		15.443 15.521	1.00 9.93	
ATOM	303	CA	GLY	49	66.948		17.393	1.00 3.43 1.00 T.27	
ATOM	304	С	GLY	49	67.199	42.211	13.829	00 5.14	
									•

bref21	c.pdt	>		Thu	Apr	25	12	: 27	:47	1996		5	
ATOM	305	0 0	SLY	49	6	7.2	94	43.3	396	19.152	1.00	3.06	5
ATOM			PRO	50	6	7.2	74	41.2		19.732		4.49	7
ATOM		CD F	PRO	50		7.1		39.		19.536	1.00	2.00	5
ATOM			PRO	50		7.5		41.5		21.135	1.00	2.99 3.97	e e
ATOM	_		PRO	50		7.5 7.9		40.1		21.762 20. 6 32	1.00	2.00	5
ATOM			PRO	50 50		8.8		42.		21.315	1.00	4.87	ર્ક
ATOM	311 312		PRO PRO	50		58.9		43.		22.217	1.00	7.36	3
MOTA MOTA	313		GLY	51		59.7		42.		20.403	1.00	5.60	7
ATOM	314		GLY	51		71.0		42.		20.477	1.00	2.83	÷.
ATOM	315		GLY	51	-	70. 9	91	44.	263	20.103	1.00	3.36	\$
ATOM	316		GLY	51		72.0		44.		19.956	1.00	5.85	÷ 7
ATOM	317		ASN	52		69.7		44.		19.968	1.00	2.00	5
MOTA	318		ASN	52		69.6 68.5		46. 46.		19.604 18.633	1.00	2.00 3.33	5
ATOM	319		ASN ASN	52 52		68.7		47.		17.666	1.00	7.97	દ
MOTA MOTA	320 321	OD1		52		69.2			311	16.538		12.55	કે
ATOM	322	ND2		52		68.4			753	18.079	1.00	10.05	7
ATOM	323	С	ASN	52		69.5	05	47.	144	20.797	1.00	3.59	5
ATOM	324	0	ASN	52		69.5			359	20.638	1.00	2.00	5
ATOM	325	N	TYR	53		69.2			573	21.985	1.00	5.70	7
MOTA	326	CA	TYP.	53		69.1			350	23.229	1.00	5.58 5.70	ē S
MOTA	327	CB	TYP	53		67.			412 547	23.770 22.768	1.00	4.84	Ę
ATOM	328	CG	TYP.	53 53		66.0			414	22.188	1.00	6.02	ě
ATOM ATOM	329 330	CD1	TYF. TYF.	53		65.6			495	21.282	1.00	5.48	ē.
MOTA	331	CD2		53		66.			789	22.405	1.00	5.30	÷
ATOM	332		TYP	53		65.3	118	48.	. 891	21.495	1.00	6.56	÷
ATOM	333	CZ	TYP.	53		64.			.729	20.929	1.00	8.17	÷
ATOM	334	OH	TYF.	53		63.			.767	19.987		12.54	3
MOTA	335	C	TYR	53		69.			. 667	24.308	1.00	3.83 4.09	ર્ગ ક
ATOM	336	0	TYR	53 54		70. 70.			.465 .428	24.245 25.346	1.00	3.81	7
ATOM	337 338	N CA	SEP.	54		70.			. 921	26.501	1.00	6.59	ē
ATOM ATOM	339	CB	SER	54		72.			. 682	26.710	1.00	8.72	6
MOTA	340	OG	SEP	54			405		.867	26.341	1.00	13.32	3
ATOM	341	С	SER	54		70.	077	47	.035	27.726	1.00	4.52	÷
ATOM	342	0	SER	54			495		.089	27.982	1.00	5.58	3
ATOM	343	N	PHE	5 5			931		.926	28.443	1.00	3.52	7
MOTA	344	CA	PHE	55			095		.878	29.641	1.00	3.38 6.11	6
MOTA	345	CB	PHE	55			141 052		.676 .700	29.574 30.596	1.00	6.96	ó
ATOM	346	CG	PHE	55 55			741		.865			10.17	é
ATOM ATOM	347 348		PHE	55			330		.547			8.73	÷
ATOM	349		PHE	5.5			713		.879		1.00	12.64	- 5
ATOM	350		PHE	55		66.	317		.561			8.02	÷
ATOM	351	CZ	PHE	55			.007		1.728			8.93	÷
MOTA	352	С	PHE	5.5			. 942		.779			2.90	5
ATOM	353	9	PHE	55			476		710			2.00 2.00	3
ATOM	354	N	SER	56			.083 .854		5.892 5.862				ē
MOTA MOTA	355 356	CA CB	SER Ser	56 56			.159		7.651				÷
ATOM	357		SER	56			. 950		3.939				5
ATOM	358		SER	56		70	.089	4	7.214	34.108			÷
ATOM	359		SER	56			.080		7.943				3
ATOM	350		TYR	57			.548		6.63				
MOTA	361		TYR	57			.915		6.85				÷
MOTA	362		TYR	57			.091		5.62: 4.33				4
ATOM	363		TYR 1 TYR	57 57			.254		3.83				Ę
ATOM ATOM	364 365		1 TYR	5	,		.86		2.58				÷
MOTA	366		2 TYR	57			.11		3.56				
ATOM	367		2 TYR	5			.72		2.31			2.48	-5
ATOM	368			5.			.09		1.83				đ
MOTA	369				-		. 67		0.59				:
MOTA	370		TYR	5.			.88		7.25			10.04	÷
ATOM	371		TYR	5			2.09 3.35		7.18 7.78			0 11.97 C 11.03	3
ATOM	37: 37:		GLN GLN	5) 5)			.18		8.14				
MOTA MOTA	37.			5			.61		9.59			0 10.64	
ATOM	37			5			2.16		0.09		2 1.0	0 13.28	.5
ATOM	37			5	ε	72	2.82	7 5	1.43	6 40.95		0 13.57	-5
ATOM	37		1 GLN	5			2.16		2.47			0 15.62	
MOTA	37		2 GLN	5			4.14		1.43			0 14.36	
ATOM	37 38		GLN	5 5			0.43 9.48		:7.88 18.58				
ATOM ATOM	38		GLN LEU				0.77		16.79				
MOTA	38				ģ		0.18		46.43				

bref21	c.pc	i b		Thu	Apr 25 1	2:27:47	1996	6	
ATOM	383	СВ	LEU	59	70.534	44.993	43.313	1.00 4.10	Ę.
ATOM	3B4	CG	LEU	59	69.811	44.344	44.446	1.00 2.46	ē
ATOM	3B5		LEU	59	68.343	44.461	44.227	1.00 3.98	5
ATOM	386		LEU	5 9	70.246	42.909	44.462	1.00 6.03	÷
MOTA	387	С	LEU	59	70.926	47.335	43.995	1.00 9.36	5
ATOM	388	0	LEU	59	72.135	47.210	44.085	1.00 9.93	3
ATOM	389	N	GLU	60	70.227	48.253	44.667	1.00 11.94	7
ATOM	390	CA	GLU	60	70.844	49.221	45.603	1.00 13.27	5
ATOM	391	CB	GLU	60	69.852	49.697	46.643	1.00 14.05	ó
ATOM ATOM	392	CC	GLU	60	70.448	50.769	47.531	1.00 15.91	5
ATOM	393 394	CD	GLU	60 60	69.443 69.263	51.351	48.510	1.00 16.83	5
ATOM	395		GLU	60	68.852	50.755	49.607	1.00 16.52	â
ATOM	396	C	GLU	60	72.159	52.410 48.859	48.181 46.315	1.00 15.77	9
ATOM	397	ō	GLU	60	72.200	47.971	47.189	1.00 14.73	6
ATOM	398	N	ASP	61	73.193	49.638	45.973	1.00 14.00 1.00 16.22	8 7
ATOM	399	CA	ASP	61	74.569	49.501	46.452	1.00 17.32	6
ATOM	400	CB	ASP	61	74.624	49.151	47.930	1.00 22.61	5
ATOM	401	CG	ASP	61	74.287	50.345	48.814	1.00 26.60	5
ATOM	402		ASP	61	74.282	50.144	50.054	1.00 30.15	ā
ATOM	403		ASP	61	74.036	51.470	48.271	1.00 27.62	3
ATOM	404	c	ASP	61	75.390	48.539	45.610	1.00 16.14	ó
MOTA	405	Ö	ASP	61	76.582	48.742	45.423	1.00 16.58	3
ATOM ATOM	406 407	N CA	GLU	62	74.758	47.476	45.130	1.00 14.78	7
ATOM	108	CB	GLU	62 62	75.402 74.418	46.524	44.223	1.00 13.68	5
ATOM	409	CG	GLU	62	74.592	45.359 44.612	43.931	1.00 15.90	5
ATOM	410	CD	GLU	62	73.574	44.998	42.585 41.452	1.00 20.15	é
ATOM	411		GLU	62	73.324	46.202	41.202	1.00 18.81 1.00 19.09	5
ATOM	412		GLU	62	73.047	44.078	40.788	1.00 19.09	8 3
ATOM	413	C	GLU	62	75.709	47.363	42.947	1.00 17.28	5
MOTA	414	0	GLU	62	75.069	48.402	42.704	1.00 10.33	3
MOTA	415	N	PRO	63	76.744	46.984	42.173	1.00 9.01	7
MOTA	416	CD	PRO	63	77.785	45.973	42.435	1.00 9.66	6
MOTA	417	CA	PRO	63	77.069	47.740	40.959	1.00 8.47	ϵ
ATOM	418	CB	PRO	63	78.517	47.322	40.691	1.00 5.33	5
ATOM	419	CG	PRO	63	78.504	45.895	41.103	1.00 7.09	6
ATOM ATOM	420 421	C	PRO	63	76.146	47.407	39.779	1.00 6.19	5
ATOM	422	и О	PRO TRP	63 64	75.473 76.119	46.366	39.775	1.00 4.91	8
ATOM	423	CA	TRP	64	75.298	48.300 48.092	38.788	1.00 3.37	7
MOTA	424	CB	TRP	64	75.441	49.259	37.613 36.645	1.00 2.00 1.00 2.40	5 5
ATOM	425	CG	TRP	64	74.591	50.490	36.923	1.00 2.40 1.00 2.00	5 5
ATOM	426	CD2	TRF	54	73.181	50.651	36.678	1.00 2.00	5
MOTA	427	CE2	TRP	64	72.845	51.972	27.050	1.00 2.28	é
MOTA	428		TRP	64	72.174	49.811	36.186	1.00 2.18	÷
ATOM	429	CD1		54	75.027	51.682	37.410	1.00 2.00	5
ATOM	430	NE1		54	73.995	52.573	37.487	1.00 2.00	7
ATOM	431	CZ2		64	71.537	52.476	36. 95 0	1.00 2.00	÷
MOTA	432	CZ3	TPP	54	70.878	50.314	36.087	1.00 2.49	ó
ATOM ATOM	433		TRP	64	70.575	51.636	36.471	1.00 2.00	6
	434	c	TPP	64 64	75.700	46.815	36.903	1.00 2.00	á
atom atom	435 436	N N	TRP LYS	64 65	76.877 74.704	46.528	26.736	1.00 2.00	3
ATOM	437	CA	LYS	65 65	74.704	46.036 44.793	36. 524 35. 8 03	1.00 2.00 1.00 2.00	7
ATOM	438	CB	LYS	55	74.603	43.597	26.668	1.00 2.00 1.00 2.61	5
ATOM	439	cs	LYS	65	75.611	43.306	37.673	1.00 3.35	5 5
ATOM	440	. CD	LYS	65	75.207	42.082	38.401	1.00 4.33	÷
ATOM	441	CE	LYS	55	76.204	41.795	39.488	1.00 10.13	5
ATOM	442	NZ	LYS	65	76.452	43.031	40.293	1.00 15.09	7
ATOM	443	C	LYS	55	74.017	44.725	24.584	1.00 2.00	5
ATOM	444		LYS	55	73.125	45.534	34.416	1.00 2.81	3
ATOM	445	22	LEU	56	74.201	43.692	33.780	1.00 2.51	7
ATOM ATOM	446	CA	LEU	6 6	73.421	43.532	32.558	1.00 3.38	÷
ATOM	447 448	OB OG	LEU LEU	55 44	74.342	43.586	21.340	1.00 2.07	-
ATOM	449		LEU	56 56	75.135 76.363	44.851	31.138	1.00 2.42	÷
ATOM	450		LEU	າຄ ວິ6	74.327	44.485	30.416	1.00 5.47	÷
ATOM	451	202	LEU	າຍ ຄໍຄົ	72.651	45.980 42.234	30.383	1.00 2.99	5
ATCM	452	-	LEU	56	73.125	41.195	32.492 32.943	1.00 3.16 1.00 2.56	5 A
ATOM	453	N	CYS	57	71.479	42.283	31.385	1.00 2.56 1.00 4.64	
ATOM	454	CA	CYS	57	76.686	41.090	31.708	1.00 8.30	5
ATOM	455	0	CYS	5 7	70.569	40.952	30.191	1.00 9.34	4
ATOM	456	÷	CYS	5 T	70.506	41.980	29.512	1.00 11.12	.3
ATOM	457	CB	27.3	57	69.331	41.275	32.363	.0C 9.6B	;
MOTA	453	3G	CYS	67	58.297	39.785	32.300	1.00 9.98	1.5
MOTA MOTA	459 460	N CA	ARG	÷6	76.672	39.729	29.649	1.00 10.38	•
	7 30	CA	AF.G	6 E	70.567	39.534	28.187	00 11.77	5

bref21	.c.pdb	Thu	Apr 25 1	2:27:47	1996	7	
ATOM	461 CB AF	G 68	71.380	38.359		1.00 15.15	ŧ
ATOM	462 CG AF		71.366				ŧ
ATOM	463 CD AF		71.858	-		1.00 21.17	<u> </u>
ATOM	464 NE AF		71.010			1.00 25.20 1.00 27.66	Ę
ATOM	465 CZ AF		71.437 72.710			1.00 28.62	÷
ATOM	466 NH1 AF		70.601	33.818		1.00 27.68	-
ATOM	467 NH2 AF	KG 68.	69.143	39.327	27.751	1.00 9.76	÷
ATOM ATOM		RG 68	68.449		28.317	1.00 9.75	=
ATOM		EU 69	68.762		26.684	1.00 8.16	
ATOM		EU 69	67.428		26.131	1.00 5.24	€ €
ATOM	*	EU 69	67.137		25.328	1.00 4.64 1.00 5.82	Ę
MOTA		EU 69	67.431 67.302		25.960 25.026	1.00 9.48	ž.
ATOM	474 CD1 L		66.498		27.111	1.00 9.06	÷
ATOM	475 CD2 L 476 C L	EU 69	67.222		25.221	1.00 6.45	÷
atom Atom		EU 69	68.175		24.655	1.00 6.60	=
ATOM		IS 70	65.947	38.430	25.133	1.00 6.17	•
ATOM		IS 70	65.448		24.296	1.00 4.34	•
ATOM		IS 70	64.792		25.103	1.00 3.32	÷
ATOM		is 70	65.759		25.871 25.460	1.00 4.94 1.00 7.46	•
ATOM	482 CD2 H		66.779 65.759		27.243	1.00 8.83	A Lowert
ATOM	483 ND1 H		66.738		27.650	1.00 9.22	÷
ATOM	484 CE1 H	_	67.372		26.586	1.00 6.78	7
MOTA MOTA		IS 70	64.40		23.546	1.00 6.62	- 5
ATOM		IIS 70	64.12	9 39.240	23.863	1.00 7.52	:
ATOM		ILN 71	63.87		22.520	1.00 10.06	
ATOM		SLN 71	62.82		21.676	1.00 12.44	÷
MOTA		ILN 71	63.44		20.442	1.00 12.64	ξ ξ
MOTA		ILN 71	62.52		19.675 18.423	1.00 11.98	÷
ATOM		SLN 71	63.19 63.25		18.185	1.00 14.18	ŧ
ATOM	493 OE1 0 494 NE2 0		63.74		17.638	1.00 13.04	7
atom atom		SLN 71	61.86		21.278	1.00 14.54	÷
ATOM		GLN 71	62.29		20.828	1.00 13.15	3
ATOM		ALA 72	60.57	6 37.148	21.510	1.00 16.60	7
ATOM		ALA 72	59.54		21.222	1.00 17.29	é
MOTA		ALA 72	59.10		22.513	1.00 18.25	6
ATOM		ALA 72			20.552 20.890	1.00 17.09	=
ATOM		ALA 72 PRO 73			19.535	1.00 15.70	= 7
ATOM		PRO 73 PRO 73			18.833	1.00 15.56	÷
ATOM ATOM		PRO 73			18.835	1.00 14.26	- 5
ATOM		PRO 73	56.53		17.608	1.00 14.62	4 5
MOTA	506 CG	PRO 73			18.096	1.00 14.52	•
ATOM	507 0	PRO 73			19.707	1.00 13.69	₹ }
MOTA	508 0	PRO 73	_			1.00 12.65	:
ATOM	509 N 510 CA	THR 74					
ATOM ATOM	510 CA 511 CB	THR 7					÷
ATOM	512 OG1				21.092	1.00 12.22	3
ATOM	513 CG2	_	\$ 51.7	90 39.484			÷
ATOM	514 C	THR 7					•
MOTA	515 O	THR 7					3
MOTA	516 N	ALA 7					÷
MOTA	517 CA	ALA 7					
ATOM	518 °CB 519 °C	ALA 7					ŧ
MOTA MOTA	520 0	ALA 7				1.00 12.33	=
ATOM	521 N	ARG 7		83 38.410	18.545		
ATOM	522 CA		6 49.1			1.00 10.37	:
MOTA	523 CB		6 48.8				:
ATOM	524 CG		6 47.7				:
MOTA	525 CD		6 47.9 6 47.2				-
MOTA	526 NE 527 CZ		6 47.2 6 47.7				:
MOTA MOTA			6 48.				-
MOTA			6 47.0				-
MOTA	530 0		50.0	026 40.04	2 15.64	1 1.00 12.35	
ATOM	531	ARG	76 49.				-
MOTA	532 N		51.2			8 1.00 12.77	
ATOM	533 CA		52.				:
ATOM	534 C		77 53.0 77 53.0				
ATOM ATOM			7. 53. 78 53.				
ATOM			78 54.				
ATOM			78 53.				

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ATOM	539	С	ALA	78	55.263	41.329	18.357	1.00 11.11	6
ATOM	540	0	ALA	78	55.080		18.495	1.00 13.01	§
ATOM	541	N	VAL	79	56.418		18.640	1.00 9.69	7
ATOM	542	CA	VAL	79	57.546		19.192	1.00 7.82	5
MOTA	543	CB	VAL	79	58.844		18.354	1.00 6.05	5
MOTA	544	CG1	VAL	79	58.706	40.741	17.024	1.00 6.29	€
ATOM	545		VAL	79	59.135	42.848	18.171	1.00 5.80	ó
ATOM	546	c	VAL	75	57.78€		20.672	1.00 5.75	ΰ
ATOM	547	0	VAL	79	57.633		21.125	1.00 4.75	Ē
ATOM	548	N	ARG	80	58.207		21.403	1.00 4.34	7
ATOM ATOM	549 550	CA CB	ARG ARG	80 80	58.420 57.507		22.813 23.550	1.00 7.09	6
ATOM	551	CG	ARG	80	57.465		25.052	1.00 B.65 1.00 7.34	6 6
ATOM	552	CD	ARG	BC	56.674		25.630	1.00 6.89	5
ATOM	553	NE	ARG	80	55.272		25.237	1.00 6.67	7
ATOM	554	CZ	ARG	80	54.415	37.809	25.313	1.00 4.11	5
ATOM	555		ARG	80	54.829		25.743	1.00 5.04	7
ATOM	556	NH2		80	53.142		25.063	1.00 2.00	7
ATOM	557	C	ARG	80	59.846		23.297	1.00 5.10	ó
ATOM	558	0	ARG	80	60.466		23.114	1.00 3.87	8
ATOM ATOM	559 560	N CA	PHE PHE	81 81	60.346		23.951	1.00 4.32	7
ATOM	561	CB	PHE	91	61.688 62.385		24.488	1.00 5.56	6
ATOM	562	CG	PHE	81	62.744		22.915	1.00 4.97	6
ATOM	563	CD1		81	61.86		22.091	1.00 5.07 1.00 6.98	é é
ATOM	564	CD2		8:	63.947		22.409	1.00 7.17	6
MOTA	565	CEL		81	62.164		20.763	1.00 7.58	5
ATOM	566	CE2	PHE	9:	64.27	42.908	21.086	1.00 10.89	6
ATOM	567	CZ	PHE	a 1	63.374	43.594	20.251	1.00 10.08	6
MOTA	568	С	PHE	81	61.54		25.955	1.00 7.23	6
ATOM	569	0	PHE	81	60.725		26.604	1.00 8.68	ā
ATOM	570	N	TRP	82	62.301		26.469	1.00 7.82	7
ATOM ATOM	571 572	CA CB	TRP TRP	82 82	62.263 61.25		27.891	1.00 8.83	ક
ATOM	573	CG	TRP	82	61.585		28.199 27.697	1.00 9.85 1.00 12.09	6 6
ATOM	574	CD2		82	62.23		28.428	1.00 12.03	6
ATOM	575	CE2		82	62.328		27.577	1.00 13.27	ě
ATOM	576	CE3		82	62.74		29.722	1.00 15.01	ś
ATOM	577	CD1	TRP	32	61.30	36.888	26.453	1.00 14.64	÷
MOTA	578	NE1	TRF	82	61.75	35.581	26.378	1.00 12.57	7
ATOM	579		TRF	32	62.91		27.987	1.00 17.05	5
ATOM	580	CZ3	TRF	82	63.33		30.137	1.00 16.75	5
ATOM	581		TRF	82	63.41		29.272	1.00 17.82	5
ATOM	582	C	TRP	82	63.65		28.371	1.00 8.05	6
ATOM ATOM	583 584	N O	TRP	82 83	64.60 63.76		27.623 29.635	1.00 7.22 1.00 7.16	3
ATOM	585	CA	CYS	83	65.02		30.282	1.00 5.52	6
ATOM	586	С	CYS	33	64.63		31.702	1.00 4.93	÷
ATOM	587	0	CYS	88	63.73	7 38.969	32.271	1.00 5.95	ā
MOTA	588	CB	CYS	33	66.02	6 39.909	30.319	1.00 7.79	5
ATOM	589	SG	CYS	33	66.43		31.992	1.00 15.35	15
ATOM	590	N	SER	34	65.24		22.258	1.00 3.11	7
ATOM	591	CA	SER SER	84	64.90		33.610	1.00 4.32	5
ATOM ATOM	592 593	CB OG	SEP.	94 84	64.39 65.09		33.658 32.731	1.00 5.70	÷
ATOM	594	C.	SER	84	66.12		34.483	1.00 12.40	3 6
ATOM	595	Ö	SER	84	67.17		34.190	1.00 11.62	3
ATOM	596		LEU	3.5	66.00		35.546	1.00 7.67	7
MOTA	597	CA	LEU	2.5	67.11		36.457	1.00 4.58	5
ATOM	598	CB	LEU	85	66.67		37.546	1.00 3.56	5
ATOM	599	CG	LEU	3.5	66.73		37.197	1.00 5.43	÷
ATOM	600		LEU	3.5	67.01		38.482	1.00 7.87	5
MOTA	601		LEU	3.5	67.84		35.232	1.00 5.46	÷
ATOM	602	5	LEU	85	67.70		27.110	1.00 5.00	ŧ
ATOM	603) N	LEU	3.5	67.00 69.02		3 ? . 352	1.00 9.20	•
MOTA MOTA	604 605	N CD	PRO	36 36	69.95		37.388 35.989	1.00 5.88	7 5
ATOM	606	CA	PRC	36	69.76		38.036	1.00 6.07	5
ATOM	607	CB	PRC	86	71.21		37.921	1.00 3.16	- 7 - 5
ATOM	608	CG	PRC	36	71.20		36.772	1.00 5.18	3
ATOM	609	C	PRC	36	69.33		39.515	1.00 3.99	-5
ATOM	610	0	PRO	96	59.14	3 36.847	40.187	1.00 4.26	-3
ATOM	611	N	THR	3-	69.22		40.029	1.00 4.59	7
atom atom	612	CA	THR	÷-	68.79		41.394	1.00 5.71	:
MOTA	613 614	CB OG1	THR THR	87 87	68.96 68.49		41.727	1.00 6.02	- 6
ATOM	615		THR	5 T	68.14		40.607 42.975	1.00 9.30	:3 -5
ATOM	616	c	THR	87	69.35		42.531	1.00 7.78	.5

ATOM 617 0 THR 81	bref21	c.pdb	Thu Ap	r 25 12:	27:47 1	996	9
ATOM 618 N ALA 88 70.661 35.474 42.561 00 8.99 4.704	n TOM	617 O THR	87	68.606 3	5.730 43		_
ATOM 619 CA ALA 88							
ATOM 620 CB ALA 88 71.694 72.812 35.1.10 43.497 1.00 10.897 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0			88				
ATOM 621 C ALA 88 10.324 38.573 44.247 1.00 10.83 10.84				_			
ATOM 622 C ALA SE							••
ATOM 623 CA SAP 89 65.33 39.470 42.397 1.00 8.96 6 ATOM 624 CA SAP 89 70.047 39.911 40.922 1.00 7.68 6 ATOM 626 CB SAP 89 71.563 39.915 40.788 1.00 6.73 6 ATOM 627 ODI ASP 89 72.319 40.224 41.720 1.00 8.92 6 ATOM 628 OD2 SAP 89 72.319 40.224 41.720 1.00 8.92 6 ATOM 628 OD2 SAP 89 72.319 40.224 41.720 1.00 8.92 6 ATOM 628 OD2 SAP 89 72.319 40.224 41.720 1.00 8.92 6 ATOM 630 CA SAP 89 67.668 40.880 42.522 1.00 9.65 6 ATOM 631 N THR 90 66.101 38.724 43.034 1.00 7.69 7 ATOM 631 CA THR 90 66.010 38.724 43.034 1.00 7.69 7 ATOM 632 CA THR 90 66.010 38.724 43.039 1.00 5.03 8.54 64 7 ATOM 634 CGI THR 90 65.983 77.603 42.898 1.00 3.00 8.87 6 ATOM 635 CGZ THR 90 65.464 33.790 45.335 1.00 11.62 5 ATOM 636 CG THR 90 65.464 33.790 45.335 1.00 11.62 5 ATOM 636 CG THR 90 65.464 33.790 45.335 1.00 11.62 5 ATOM 636 CG THR 90 66.464 33.790 45.335 1.00 11.62 5 ATOM 637 C THR 90 66.464 33.790 45.335 1.00 11.62 5 ATOM 638 N SER 91 66.424 40.043 45.479 1.00 7.49 7 ATOM 640 CG SER 91 66.494 41.778 41.788 1.00 9.23 6 ATOM 641 CG SER 91 66.494 41.788 47.488 1.00 9.23 6 ATOM 642 CG SER 91 66.497 42.197 46.263 1.00 9.23 8 ATOM 640 CG SER 91 66.497 40.138 47.488 1.00 9.38 7 ATOM 640 CG SER 91 66.497 40.138 47.488 1.00 9.23 8 ATOM 640 CG SER 91 66.497 40.108 41.255 47.03 1.00 8.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 10.62 2 ATOM 640 CG SER 91 64.779 42.197 40.203 1.00 8.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 0.70 3.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 0.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 0.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 0.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 0.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 0.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 0.55 5 ATOM 640 CG SER 92 63.000 41.671 43.339 1.00 0.55 5 ATOM 640 CG SER 92 63.000 41.671 43.399 48.744 1.00 0.00 6 ATOM 640 CG SER 92 61.620 40.702 40.003 1.00 7.73 5 ATOM 640 CG SER 92 61.620 40.702 40.003 1.00 7.73 5 ATOM 640 CG SER 92 61.620 40.702 40.003 1.00 7.73 5 ATOM 640 CG SER 92 60.004 40.00	MOTA						
ATOM 624 CG ASP 89 10.0047 39.911 40.992 1.00 7.68 5 ATOM 626 CG ASP 89 11.563 39.915 40.992 1.00 7.68 5 ATOM 627 CDI ASP 89 72.319 40.224 41.720 1.00 8.92 2 ATOM 628 CD2 ASP 89 72.012 39.646 29.667 1.00 6.25 3 ATOM 629 C ASP 89 68.141 39.746 42.654 1.00 9.62 5 ATOM 621 N THR 90 67.420 38.724 43.094 1.00 7.69 7 ATOM 621 N THR 90 67.420 38.724 43.094 1.00 7.69 7 ATOM 631 N THR 90 66.1010 38.866 43.359 1.00 5.03 5 ATOM 632 CG THR 90 65.989 37.603 42.898 1.00 3.78 5 ATOM 633 CB THR 90 65.983 37.603 42.898 1.00 3.78 5 ATOM 636 C THR 90 65.965 38.864 43.455 1.00 2.18 5 ATOM 637 O THR 90 64.632 38.004 42.359 1.00 1.02 7.69 7 ATOM 638 N SEP 91 66.6610 38.004 42.31 1.00 1.62 8 ATOM 637 O THR 90 64.632 38.004 42.31 1.00 1.62 8 ATOM 638 N SEP 91 66.264 04.34 46.87 1.00 7.21 6 ATOM 630 CS SER 91 66.264 04.34 46.87 1.00 7.21 6 ATOM 641 OS SER 91 66.264 04.34 46.87 1.00 9.23 6 ATOM 642 C SER 91 64.770 41.178 47.488 1.00 9.38 8 ATOM 643 CS SER 91 64.770 41.072 41.478 1.00 9.38 8 ATOM 646 CB SER 91 64.770 41.672 40.03 1.00 8.55 6 ATOM 646 CB SER 92 64.797 41.029 48.125 1.00 8.55 7 ATOM 646 CB SER 92 62.022 40.702 49.003 1.00 7.73 5 ATOM 646 CB SER 92 62.022 40.702 49.003 1.00 7.73 5 ATOM 646 CB SER 92 62.022 40.702 49.003 1.00 7.73 5 ATOM 646 CB SER 92 62.022 40.702 49.003 1.00 7.73 5 ATOM 650 CB PHE 93 63.600 43.548 44.805 1.00 9.02 8 ATOM 650 CB PHE 93 63.600 43.551 49.764 1.00 2.00 6 ATOM 650 CB PHE 93 64.601 43.484 63.550 60 9.02 2 ATOM 664 CB SER 92 62.022 40.702 49.003 1.00 7.73 5 ATOM 650 CB PHE 93 64.787 44.887 60.90 1.00 7.73 5 ATOM 650 CB PHE 93 64.787 40.187 44.881 1.00 9.02 2.00 6 ATOM 650 CB PHE 93 64.787 40.187 44.881 1.00 2.00 6 ATOM 650 CB PHE 93 64.787 40.187 44.881 1.00 2.00 6 ATOM 650 CB PHE 93 64.787 40.187 44.881 1.00 2.00 6 ATOM 650 CB PHE 93 64.787 40.00 44.94 4							00 8.96 5
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ATOM 678 CG LEU 96 65.571 45.607 40.411 1.00 2.00 6 ATOM 679 CD1 LEU 96 66.945 45.060 40.642 1.00 2.00 6 ATOM 680 CD2 LEU 96 64.648 44.446 40.315 1.00 2.00 6 ATOM 681 C LEU 96 65.712 48.886 40.816 1.00 6.21 6 ATOM 682 C LEU 96 64.639 49.309 40.367 1.00 5.02 7 ATOM 683 N GLU 97 66.881 49.355 40.416 1.00 3.18 7 ATOM 685 CB GLU 97 67.000 50.324 39.336 1.00 3.49 6 ATOM 685 CB GLU 97 68.315 51.069 39.476 1.00 10.17 7 ATOM 686 CG GLU 97 68.315 51.069 39.476 1.00 10.17 7 ATOM 687 CD GLU 97 67.806 53.335 23.676 1.00 12.04 ATOM 688 0E1 GLU 97 67.806 53.335 23.676 1.00 12.04 ATOM 689 0E2 GLU 97 67.252 52.737 37.691 1.00 14.20 ATOM 690 C GLU 97 66.959 49.610 37.987 1.00 3.71 ATOM 691 C GLU 97 66.959 49.610 37.987 1.00 3.71 ATOM 692 N LEU 98 66.083 50.053 37.101 1.00 3.76 ATOM 693 CA LEU 98 66.083 50.053 37.101 1.00 3.77						41.543	
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ATOM	695	CG	LEU	98	64.	366	47.487	35.686	1.00	3.97	Ę
MOTA	696	CD1	LEU	98	62.		47.080	35.721	1.00	9.15	5
ATOM	697	CD2	LEU	98	65.	203	46.309	35.266	1.00	3.89	į.
ATOM	698	С	LEU	98	66.	141	50.388	24.676	1.00	9.74	ŝ
ATOM	699	0	LEU	98	65.	751	51.556	34.781		11.17	3
ATOM	700	N	ARG	99	66.	814	49.945	23.621	1.00	7.82	2
ATOM	701	CA	ARG	99	67.	050	50.799	32.467	1.00	8.42	ē.
ATOM	702	CB	ARG	99	68.		51.701	32.680	1.00	9.99	<i>₹</i>
ATOM	703	CG	ARG	99	68.		52.571	33.915	1.00	13.57	÷.
ATOM	704	CD	ARG	99	69.		53.483	33.832	1.00	15.65	5
MOTA	705	NE	ARG	99	70.		52.717	33.766		21.42	7
ATOM	706	CZ	ARG	99	71.		52.634	32.709	1.00	23.75	5
ATOM	707		ARG	99	71.		53.271	31.557	1.00	25.09	7
ATOM	708		ARG	99	72.		51.921	32.818	1.00	24.11	7
ATOM	709	C	ARG	99	67.		50.002	31.174	1.00	7.84	5
ATOM	710	0	ARG	99	68.		49.159	31.118	1.00	8.53	3
ATOM	711	N	VAL	100	66.		50.307	30.136	1.00	5.56	7
ATOM	712	CA	VAL	100	66.		49.664	28.852	1.00	5.54	5
ATOM	713	CB	VAL	100	65.		49.097	28.397	1.00	8.61	5
ATOM	714	CG1	VAL	100	65.		48.467	27.008	1.00	7.63	ē
ATOM	715	CG2	VAL	100	64.1		48.100	29.419	1.00	7.70	5
ATOM ATOM	716 717	0	VAL	100	67.		50.745	27.877	1.00	6.61	5
ATOM	718	N	VAL	100	66.		51.831	27.819	1.00	3.63	3
ATOM	719	CA	THR THP	101 101	68.; 68.		50.490	27.156	1.00	7.98	7
ATOM	720	CB	THP.	101	70.		51.483	25.193	1.00	10.18	ō
ATOM	721	OG1	THP.	101	70.		52.277	26.748	1.00	8.43	÷
ATOM	722	CG2	THE	101	69.		51.629 53.663	27.908 27.148	1.00	13.91 11.20	3
ATOM	723	c	THR	101	69.		50.926	24.792	1.00		-
ATOM	724	Ö	THR	101	69.		49.758			11.66	é
ATOM	725	N	ALA	102	68.		51.752	24.645 23.767		11.61 12.50	9 7
ATOM	726	CA	ALA	102	69.		51.369	22.386		14.07	÷
ATOM	727	СВ	ALA	102	68.		52.465	21.399		14.73	5
ATOM	728	C	ALA	102	70.		51.154	22.249		13.24	5
ATOM	729	0	ALA	102	71		51.752	23.012		12.22	a
ATOM	730	N	ALA	103	71.		50.332	21.270		12.73	7
ATOM	731	CA	ALA	103	72.		50.004	21.021		13.74	5
ATOM	732	CB	ALA	103	72.		48.712	20.183		15.06	
MOTA	733	С	ALA	103	73.	250	51.173	20.338		14.07	5
ATOM	734	0	ALA	103	73.	958	51.013	19.345	1.00	16.53	а
ATOM	735	N	SER	104	73.	105	52.341	20.931	1.00	12.51	7
ATOM	736	CA	SEP.	104	73.	673	53.569	20.440	1.00	10.25	÷
ATOM	737	CB	SEP.	104	72.	834	54.066	19.266	1.00	9.41	÷
ATOM	738	OG	SER	104	71.		54.033	19.565	1.00	8.47	3
ATOM	739	С	SER	104	73.		54.528	21.600		11.58	÷
ATOM	740	0	SEP.	104	73.		55.746	21.412		11.80	3
ATOM ATOM	741	N	GLY	105	73.		53.964	22.770	1.00	11.41	7
ATOM	742 743	CA C	GLY	105	73.		54.747	23.976	1.50	12.64	÷
ATOM	744	0	GLY	105 105	71. 71.		55.568	23.980	1.00	13.51	÷
ATOM	745	N	ALA	106	70.		56.335	24.921		15.64	3
ATOM	746	CA	ALA	106	69.		55.433	22.930		12.54	:
ATOM	747	CB	ALA	106		068	56.166	22.837		11.65	5
ATOM	748	c	ALA	106		752	56.040 55.553	21.444 23.884		13.77	ę
ATOM	749	ō	ALA	106		501	54.338	23.899		11.28	ć
ATOM	750	N	PRO	107		239	56.392	24.779	1.00	8.60	5
ATOM	751	CD	PP.C	107	68.		57.855	24.686	1.00	9.28	
ATOM	752		PRC	107		354	56.019	25.882	1.00	7.77	÷
ATOM	753	CB	PRC	127		282	57.314	25.683	1.00	8.42	- 6
ATOM	754	CG	PRO	197		302	58.359	25.605	1.00	9.15	é
MOTA	755	С	PRO	107		964	55.459	25.552	1.00	7.66	4
MOTA	756	0	PRO	107	65.	224	56.048	24.761	1.00	8.78	3
ATOM	757	N	AP.G	108	65.	595	54.353	25.196	1.00	7.20	5 -
ATOM	758	CA	ARG	108	64.	290	53.751	25.990	1.00	4.63	-5
ATOM	759	CB	ARG	108		439	52.415	25.288	1.00	7.43	-5
ATOM	760	CG	ARG	108		168	51.903	24.695	1.00	10.88	•
ATOM	761	CD	ARG	108		783	52.688	23.460	1.00	14.12	-5
MOTA	762	NE	ARG	108		461	52.318	22.964	1.00	15.25	.5 -
ATOM	763	CZ	ARG	108		086	51.084	22.550	1.00	15.01	5
ATOM	764		ARG	108		917	50.067	22.764	1.00	18.31	
ATOM	765		ARG	108		858	50.867	22.236	1.00	19.47	?
ATOM ATOM	766 767	C	ARG	108		455	53.624	27.253	1.20	5.36	-5
ATOM	768	N C	ARG	108		420	54.259	27.404	1.20	5.86	-
ATOM	769	N CA	TYR TYR	109		883	52.837	28.263	1.00	5.12	
MOTA	770	CE	TYR	109 109		1.02	52.711	29.509	1.00	5.72	•
ATOM	771	CG	TYF	109		419 455	51.350 51.024	29.631	::		1
ATOM	772		TYR	109		775	50.089	28.544	1.10	8.20	•
	-		• `		U.,	. , ,	55.009	21.303	30	11.38	- 1

bref21	c.pdb	Thu Ap	r 25 12:	27:47		11	
ATOM	773 CE1 TYR	109				•• •	5 5
ATOM	774 CD2 TYP.	109					E.
ATOM	775 CE2 TYR	109		-	7.476 6.511		5
ATOM	776 CZ TYR	109		•			ā
ATOM	777 OH TYR	109					ક
MOTA	778 C TYR	109 109			0.794 1.	00 9.59	5
MOTA	779 0 TYR 780 K HIS	110			1.835 :.	00 10.99	7
ATOM	780 N HIS 781 CA HIS	110		3.467	3.174 -	00 14.45	÷
ATOM ATOM	782 CB HIS	110				00 16.04	ş
ATOM	783 CG HIS	110				00 21.12	6 6
ATOM	784 CD2 HIS	110			25.048 1. 35.652 1.	.00 24.07	7
ATOM	785 ND1 HIS	110			36.662	.00 23.40	6
MOTA	786 CE1 HIS	110			36.321	.00 22.60	7
MOTA	787 NE2 HIS 788 C HIS	110 110			34.214 1	.00 12.21	ć
ATOM	788 C HIS 789 O HIS	110				.00 13.06	8
MOTA MOTA	790 N ARG	111				.00 11.08	7
MOTA	791 CA ARG	111		52.116		.00 10.30	6 6
ATOM	792 CB ARG	111		50.881		.00 9.90 .00 8.05	5
ATOM	793 CG ARG	111		50.590		.00 8.05 .00 8.40	5
MOTA	794 CD ARG	111	58.370 57.828	50.465 49.099		.00 8.93	7
ATOM	795 NE ARG	111	57.096	48.521		.00 8.80	6
ATOM	796 CZ ARG 797 NH1 ARG	111 111	56.822	49.182	37.840	.00 10.13	7
MOTA	797 NH1 ARG 798 NH2 ARG	111	56.585	47.308		.00 10.84	7
MOTA MOTA	799 C ARG	111	62.546	51.850		.00 11.27	ર
ATOM	800 C ARG	111	63.776	51.808		00 13.11	3 7
MOTA	801 N VAL	112	61.877	51.75B		00 11.56	6
ATOM	802 CA VAL	112	62.493	51.471		.00 12.50	5
MOTA	803 CB VAL	112	62.882 63.003	52.803 52.545		1.00 13.08	6
MOTA	804 CG1 VAL	112 112	64.235	53.354		1.00 12.31	6
ATOM	805 CG2 VAL 806 C VAL	112	61.398	50.668	40.542	1.00 7.77	5
ATOM ATOM	807 0 VAL	112	60.268	51.105		1.00 8.50	3
ATOM	808 N ILE	113	61.709	49.480		1.00- 5.20	7
ATOM	809 CA ILE	113	60.692	48.638		1.00 6.80	6 6
ATOM	810 CB ILE	113	60.223	47.527		1.00 5.60 1.00 6.45	5
ATOM	811 CG2 ILE		59.680	48.130	39.426 40.315	1.00 6.45	5
ATOM	812 CG1 ILE		61.396 61.012	46.623	39.468	1.00 9.87	6
MOTA	813 CD1 ILE		61.105	47.931	43.001	1.00 7.16	5
ATOM	814 C ILE 815 C ILE		62.141	48.234	43.572	1.00 9.02	ક
ATOM ATOM	815 C ILE 816 N HIS		60.267	47.000	43.463	1.00 2.78	7
ATOM	817 CA HIS		60.503	46.187	44.645	1.00 2.00	5
ATOM	818 CB HIS		59.793	46.758	45.860	1.00 2.00	5
ATOM	819 CG HIS		60.554	47.827	46.555 47.652	1.00 2.00	
ATOM	820 CD2 HI		61.337 60.589	47.787 49.130	46.105	1.00 4.03	5 7
ATOM	821 ND1 HI		61.368	49.850	46.891	1.00 2.34	÷
ATOM	822 CE1 HI		61.835	49.057	47.838	1.00 8.31	7
ATOM ATOM	823 NE2 HI:		59.907	44.830		1.00 2.00	÷
ATOM	825 0 HI		58.705		44.221	1.00 2.00	5
ATOM	826 N IL	_	60.741			1.00 2.00	-
MOTA	827 CA IL		60.261			1.00 2.00 1.00 3.84	5 8
ATOM	828 CB IL		61.439			1.00 4.23	6
MOTA	829 CG2 IL		760.953 62.333			1.00 2.00	
ATOM	830 · CG1 IL	E 115 E 115	63.731			1.00 2.23	
ATOM	831 CD1 IL 832 C IL	_	59.107			1.00 3.56	
MOTA			58.294			1.00 6.91	
ATOM ATOM		_	59.013			1.00 4.63	
ATOM			57.93			1.00 5.21	
ATOM		N 116	58.31			1.00 5.33	
ATOM	837 CG A	SN 116	58.582			1.00 5.94	
MOTA			59.470			1.00 8.46	
ATOM			57.80° 56.58°			1.00 5.92	
ATOM	_	SN 116 SN 116	55.51				
MOTA MOTA		LU 117	56.66			2.00 8.30	5
MOTA MOTA	· _	LU 117	55.48	0 44.51	4 45.436		
OTA		LU 117	55.73				
ATON	4 845 CG G	LU 117	55.95				
ATO	_	LU 117	56.16				
ATO			56.64 55.81				
ATO	_	LU 117	55.11				
ATO! ATO!		LU 117	54.44				

bref21	c.pc	i b		Thu	Apr	25	12	::27:47	1996		12	
ATOM	851	N	VAL	118	5	5.47	7	43.151	43.523	1.00	3.55	7
ATOM	852	CA	VAL	118		5.22		42.839	42.137	1.00	2.91	
ATOM	853	CB	VAL	118	5	6.37	3	43.488	41.261	1.00	2.00	Ē
ATOM	854	CG1	VAL	118	5	7.48	4	42.519	40.942	1.00	2.85	:
ATOM	855	CG2	VAL	118	5	5.82	8	44.165	40.062	1.00	2.00	÷
ATOM	856	С	VAL	118	5	5.06	0	41.334	41.948	1.00	2.18	÷
ATOM	857	0	VAL	118	5	5.45	3	40.755	40.936	1.00	3.50	3
ATOM	858	N	VAL	119	5	4.40	4	40.716	42.919	1.00	2.79	-
ATOM	359	CA	VAL	119	5	4.15	5	39.276	42.896	1.00	3.05	:
ATOM	860	CB	VAL	119		3.77		38.736	44.305	1.00	2.45	•
ATOM	861	CG1		119		3.74		37.267	44.292	1.00	2.00	÷
MOTA	862		VAL	119		4.73		39.231	45.352	1.00	2.00	E
MOTA	863	C	VAL	119		2.99		38.960	41.945	1.00	2.00	÷
ATOM	864	0	VAL	119		2.00		39.674	41.932	1.00	2.00	3 7
ATOM	865	N	LEU	120		3.17		37.919	41.132	1.00	3.02	
ATOM	866	CA	LEU	120		2.17		37.411	40.174	1.00	2.95	ć
atom Atom	867	CB	LEU	120		2.44		37.894	38.745	1.00	5.65	á
	868	CG		120		1.49		37.332	37.674		11.07	5
ATOM ATOM	869 870		LEU LEU	120		0.12		37.938	37.790	1.00	9.95	5
ATOM	871	C	LEU	120 120		2.05 2.28		37.605	36.306		11.67	5
ATOM	872	0	LEU	120		2.98		35.887 35.241	40.262	1.00	2.40	5
ATOM	873	N	LEU	121		1.60		35.340	39.487	1.00	2.00	ě
ATOM	874	CA	LEU	121		1.62		33.924	41.250	1.00	2.39	7
ATOM	875	CB	LEU	121		1.06		33.689	41.552	1.00	2.77	5
ATOM	876	CG	LEU	121		2.05		33.227	42.964	1.00	4.57	ž.
ATOM	877	CD1	LEU	121		2.93		32.076			10.24	
ATOM	878		LEU	121		2.94			43.550		14.87	•
ATOM	879	C	LEU	121		0.97		34.328 32.995	44.501	1.00	9.45	÷.
ATOM	880	Ö	LEU	121		0.25				1.00	5.41	-
ATOM	881	N	ASP	122		1.27		33.420	39.654	1.00	7.90	3
ATOM	882	CA	ASP	122				31.709	40.672	1.00	8.57	7
ATOM	883	CB	ASP	122		0.68 1.49		30.726	39.782	1.00	6.90	é
ATOM	884	CG	ASP	122		2.70		29.421 29.437	39.773	1.00	7.76	5
ATOM	885		ASP	122		2.92		30.429	38.795 38.066	1.00	9.54	á
ATOM	886		ASP	122		3.41		28.405		1.00	9.98	5
ATOM	887	c	ASP	122		9.29		30.494	38.748		10.20	3
ATOM	888	ŏ	ASP	122		18.95		30.954	41.453	1.00	7.04	5
ATOM	889	N	ALA	123		18.46		29.813	39.568	1.00	5.44	3 7
ATOM	890	CA	ALA	123		7.10		29.562	40.010	1.00	6.22 4.76	, 5
ATOM	891	CB	ALA	123		6.18		29.374	38.839	1.00	2.00	
ATOM	892	c	ALA	123		16.98		28.398	40.954	1.00	3.93	÷
ATOM	893	0	ALA	123		17.82		27.484	40.971	1.00	5.37	5
ATOM	894	N	PRC	124		15.97		28.490	41.846	1.00	2.51	7
ATOM	895	CD	PRO	124		15.21		29.736	42.096	1.00	2.90	÷
ATOM	896	CA	PRO	124		15.65		27.478	42.845	1.00	2.91	4
ATOM	897	СВ	PRO	124		14.36		28.022	43.436	1.00	2.00	6
ATOM	898	CG	PRO	124		4.60		29.485	43.432	1.00	2.55	-
ATOM	899	С	PPC	124		15.45		26.111	42.172	1.00	2.00	÷
ATOM	900	0	PRO	124		15.28		26.022	40.966	1.00	2.00	÷
ATOM	901	N	VAL	125		15.52		25.042	42.944	1.00	2.31	-
ATOM	902	CA	VAL	125		15.34		23.715	42.381	1.00	4.06	-
ATOM	903	CB	VAL	125		46.72		23.006	42.025	1.00	2.00	÷
ATOM	904		VAL	125		47.47		23.806	40.974	1.00	2.00	•
ATOM	905		VAL	125		47.58		22.776	43.256	1.00	2.00	•
ATOM	906	С	VAL	125		44.43		22.838	43.267	1.00	5.51	:
ATOM ·	907	0	VAL	125	`2	44.00	02	23.281	44.316	1.00	6.33	:
ATOM	908	' N	GLY	126		44.06		21.661	42.768	1.00	5.23	the state of the entire
ATOM	909	CA	GLY	126	4	43.23	30	20.735	43.494	1.00	4.13	5
ATOM	910	С	GLY	12€	4	41.93	39	21.283	44.035	1.00		•
ATOM	911	O	GLY	126	4	41.58	38	20.981	45.170	1.00		=
ATOM	912	N	LEU	127	4	41.24	18	22.113	43.268	1.00		-
ATOM	913	CA	LEU	127	:	39.97	71	22.667	43.718	1.00	7.87	:
ATOM	914	CB	LEU	12-		39.59		23.949	42.935	1.00	9.72	me we we do no no
ATOM	915	CG	LEU	12-	;	38.17	7.5	24.573	43.071	1.00		5
ATOM	916		LEU	127		37.95	54	25.322	44.424	1.00		÷
ATOM	917		LEU	127	:	37.94	42	25.516	41.892		10.21	:
ATOM	918	C	LEU	12		38.84	46	21.623	43.612	1.00	6.35	:
ATOM	919	0	LEU	12-	:	38.58	85	21.083	42.538	1.00		•
ATOM	920	N	VAL	128		38.17	77	21.369	44.737	1.00		:
ATOM	921	CA	VAL	128		37.08	87	20.406	44.815	1.00		5
ATOM	922	CB	VAL	128		37.48		19.147	45.616	1.00		÷
MOTA	923		VAL	128		37.99		18.080	44.701	1.00		÷
ATOM	924		VAL	128		38.52		19.477	46.659	1.00	9.52	:
ATOM	925	Ç	VAL	128		35.86		21.001	45.470	00	5.27	÷
ATOM	926	Ö	VAL	128		35.9		21.795	45.374	1.00	5.97	÷
ATOM	927	N	ALA	129		34.69		20.574	45.031	1.00		•
ATOM	928	CA.	ALA	129		33.4	30	21.061	45.579	1.00	5.ći	÷

bref21	c.pdb		Thu	Apr 25 12	:27:47	1996	13
ATOM	929 C	B ALA	129				.00 4.36 5
ATOM	930 C	ALA	129				
ATOM	931 0		129				00 9.32 3 00 9.76 7
ATOM	932 N		130				.00 10.55
ATOM		A ARG	130	31.288 32.220			.00 11.88 6
MOTA		B ARG	130 130	31.765			.00 11.87 6
ATOM		G ARG	130	32.108			.00 15.67 5
MOTA		E ARG	130	33.351			1.00 15.76 7
ATOM		Z ARG	130	33.669	18.135		1.00 20.46 é
ATOM		H1 ARG	130	32.818	18.092		1.00 18.08 7
ATOM ATOM		H2 ARG	130	34.840	18.791		1.00 21.04
ATOM		ARG	130	30.028	19.479		1.00 10.90 5
ATOM		ARG	130	29.932	20.593		1.00 10.77 8
ATOM		N LEU	131	29.065	18.582		1.00 12. 00 7 1.00 13.66 5
ATOM	944	CA LEU	131	27.813	18.909		
ATOM	945	CB LEU	131	26.640	18.313		1.00 12.73 6 1.00 11.96 5
MOTA	-	CG LEU	131	25.301	18.517		1.00 10.47 6
MOTA		CD1 LEU	131	25.035	20.002 17.783		1.00 11.69 6
MOTA		CD2 LEU	131	24.252	18.409		1.00 13.46 6
MOTA		C LEU	131	27. 79 9 27.702	17.204	51.128	1.00 12.81 8
ATOM	-	O LEU	131	27.702	19.328	51.834	1.00 14.88 7
ATOM		N ALA	132	27.964	18.982	53.249	1.00 16.22 6
ATOM		CA ALA	132 132	28.272	20.228	54.122	1.00 14.97 6
ATOM		CB ALA	132	26.638	18.324	53.656	1.00 16.57 6
ATOM	954 955	C ALA	132	25.719	19.000	54.109	1.00 16.97 3
ATOM	955 956	N ASP	133	26.553	17.009	53.411	1.00 20.15 7
ATOM ATOM	957	CA ASP	133	25.397	16.156	53.729	1.00 22.27 5
ATOM	958	CB ASP	133	25.868	14.755	54.193	1.00 23.23 6
ATOM	959	CG ASP	133	26.187	12.783	53.024	1.00 25.72 5
ATOM	960	OD1 ASP	133	25.704	14.012	51.871	1.00 26.91 3
ATOM	961	OD2 ASP	133	26.894	12.758	53.284	1.00 25.03
ATOM	962	C ASP	133	24.655	16.814	54.885	1.00 22.10 6
ATOM	963	O ASP	133	23.575	17.415	54.715	
ATOM	964	N GLU	134	25.310	16.B02	56.037	
ATOM	965	CA GLU	134	24.742	17.410	57.211	-
MOTA	966	CB GLU	134	25.478	16.953	58.482	1.00 17.36 5 1.00 17.83 5
ATOM	967	cc cru	134	26.589	15.897	58.287 58.153	1.00 17.83 5
MOTA	968	CD GLU	134	28.003	16.514 15.726	58.020	1.00 19.82 8
ATOM	969	OE1 GLU	134	28.980 28.136	17.775	58.183	1.00 18.81 3
MOTA	970	OE2 GLU	134	24.784	18.933	57.068	1.00 17.19 5
MOTA	971	C GLU	134 134	25.842		57.197	1.00 18.37 3
MOTA	972 973	N SER	135	23.648		56.657	1.00 16.42 7
ATOM	974	CA SEP.		23.375		56.510	1.00 17.66 5
MOTA MOTA	975	CB SEP.	_	24.435		57.166	1.00 17.67 6
ATOM	976	OG SER		25.623		55.400	1.00 19.35
ATOM	977	C SER			21.443		1.00 18.19 5
ATOM	978	C SEP					1.00 17.96
ATOM	979	N GLY					1.00 19.82 7
MOTA	980	CA GLY	136	22.945			1.00 21.54 5
ATOM	981	C GLY					1.00 22.07 6
ATOM	982	o GLY					1.00 22.69 5
ATOM	983	N HIS					
MOTA	984	CA HIS					
ATOM	985	CB HIS					
ATOM	986	CG HIS					
MOTA	987	CD2 HIS					
ATOM	988						
ATOM	989				-		
MOTA	990						
MOTA	991						
MOTA	992						
ATOM ATOM	993 994						
ATOM	995						
ATOM	996					6 47.390	1.00 10.78
ATOM	997				4 23.25		
ATOM	998				23.87	7 50.15	
ATOM	999			8 29.96			
	1000			9 30.87			
ATOM					94 23.26		4 1.00 10.38
ATOM ATOM	1001	l ca va					
				9 32.53			
ATOM	1002	2 CB VA	L 13	9 32.53 9 33.71	81 22.87	77 52.62	0 1.00 7.80
ATOM ATOM ATOM ATOM	1002	2 CB VA 3 CG1 VA 4 CG2 VA	L 13 L 13 L 13	9 32.53 9 33.71 19 31.41	81 22.87 15 22.39	77 52.62 93 52.94	0 1.00 7.80 6 1.00 6.80
ATOM ATOM ATOM	1002 1002 1004 1005	2 CB VA 3 CG1 VA 4 CG2 VA 5 C VA	L 13 L 13 L 13 AL 13	19 32.53 19 33.71 19 31.41 39 33.21	81 22.83 15 22.39 49 23.09	77 52.62 93 52.94 95 49.61	0 1.00 7.80 6 1.00 6.80 5 1.00 10.04

bref2	1c.pd	ъ		Thu	Apr 25 12	: 27 : 47	1996	14	
ATOM	1007	N	LEU	140	33.975	24.194	49.372	1.00 a.25	7
ATOM	1008	CA	LEU	140	35.027	24.306	43.384	1.00 6.26	ė
ATOM	1009	СВ	LEU	140	34.986	25.673	47.761	1.00 2.05	÷
ATOM	1010	CG	LEU	140	33.726	25.968	47.000	1.00 2.00	Š
ATOM	1011	CD1		140	33.806	27.395	46.505	1.00 2.00	5
MOTA	1012	CD2	LEU	140	33.594	24.972	45.869	1.00 2.00	÷
ATOM	1013	С	LEU	140	36.354	24.170	49.069	1.00 3.88	ક
MOTA	1014	0	LEU	140	36.566	24.774	50.115	1.00 10.60	ŧ
MOTA	1015	N	ARG	141	37.278	23.481	48.409	1.00 11.34	7
MOTA	1016	CA	ARG	141	38.618	23.235	48.929	1.00 12.76	ē
MOTA	1017	CB	ARG	141	38.682	21.805	49.446	1.00 16.99	ó
ATOM ATOM	1018 1019	CD	ARG ARG	141 141	39.347	21.645	50.793	1.00 21.35	5
ATOM	1020	NE	ARG	141	40.849 41.431	21.410	50.697 52.042	1.00 24.13	5 7
ATOM	1021	CZ	ARG	141	42.344	22.314	52.482	1.00 30.00	5
ATOM	1022		ARG	141	42.821	23.266	51.673	1.00 30.75	7
ATOM	1023	NH2		141	42.727	22.282	53.773	1.00 29.95	7
ATOM	1024	C	ARG	141	39.632	23.383	47.804	1.00 13.10	6
ATOM	1025	0	ARG	141	39.289	23.227	46.639	1.00 13.55	8
MOTA	1026	N	TRP	142	40.871	23.715	48.154	1.00 11.10	7
ATOM	1027	CA	TRP	142	41.941	23.846	47.182	1.00 6.61	5
ATOM	1028	CB	TRP	142	41.754	25.107	46.354	1.00 6.92	5
ATOM	1029	CG	TRP	142	41.661	26.356	47.155	1.00 9.55	5
ATOM	1030		TRP	142	40.482	26.905	47.749	1.00 9.85	÷
ATOM	1031	CE2	TRP	142	40.852	28.094	48.397	1.00 9.31	5
MOTA	1032 1033		TRP TRF	142	39.145	26.508	47.788	1.00 10.67	5
ATOM ATOM	1033	NE1	TRP	142 142	42.671 42.196	27.216 28.267	47.456 48.209	1.00 10.90	ē
ATOM	1035	CZ2		142	39.937	28.885	49.072	1.00 11.52	5
ATOM	1036	CZ3	TRP	142	38.245	27.296	43.454	1.00 11.65	5
ATOM	1037	CH2		142	38.645	28.474	49.089	1.00 9.80	5
ATOM	1038	c	TRP	142	43.288	23.857	47.877	1.00 5.00	6
ATOM	1039	0	TRP	142	43.380	23.703	49.076	1.00 6.66	3
MOTA	1040	N	LEU	143	44.349	23.995	47.109	1.00 5.47	7
ATOM	1041	CA	LEU	143	45.700	24.039	47.656	1.00 3.56	6
ATOM	1042	CB	LEU	143	46.520	22.876	47.123	1.00 2.35	5
ATOM	1043	CG	LEU	143	46.031	21.474	47.408	1.00 2.00	6
ATOM	1044		LEU	143	46.832	20.483	46.601	1.00 2.00	6
MOTA	1045		LEU	143	46.182	21.223	48.862	1.00 2.00	é
ATOM	1046	C	LEU	143	46.310	25.326	47.158	1.00 2.00	5
ATOM ATOM	1047 1048	O N	LEU PRO	143 144	45.765 47.411	25.970 25.759	46.274	1.00 4.81	â
ATOM	1049	CD	PRO	144	48.003	25.327	47.762 49.030	1.00 2.00	7
ATOM	1050	CA	PRO	144	48.027	26.996	47.295	1.00 2.00 1.00 2.00	ē.
ATOM	1051	CB	PRO	144	48.955	27.359	43.445	1.00 2.00	5
ATOM	1052	CG	PRO	144	48.442	26.605	49.601	1.00 2.00	÷
ATOM	1053	С	PRO	144	48.821	26.750	46.011	1.00 2.00	÷
ATOM	1054	C	PRO	144	48.999	25.611	45.580	1.00 2.00	3
ATOM	1055	N	PRO	145	49.249	27.823	45.342	1.00 2.00	7
ATOM	1056	CD	PRO	145	49.058	29.249	45.645	1.00 2.00	÷
MOTA	1057	CA	PRO	145	50.022	27.643	44.113	1.00 2.72	÷
ATOM	1058	CB	PRO	145	50.532	29.053	43.839	1.00 2.80	5
ATOM	1059	CC	PRO	145	49.467	29.898	44.372	1.00 2.95	÷
MOTA MOTA	1060 1061	0 0	PRO PRO	145 145	51.178 51.875	26.696 26.899	44.455 45.448	1.00 4.71 1.00 3.80	÷
ATOM	1062	Ŋ	PRO	146	51.396	25.652	43.639	1.00 9.22	3
ATOM	1063	CD	PRO	146	50.738	25.412	42.347	1.00 5.22	÷
ATOM	1064		PRO	146	52.462	24.665	43.857	1.00 6.83	÷
ATOM	1065	CB	PRO	146	52.358	23.778	42.622	1.00 7.88	Ę
ATOM	1066	CG	PRO	146	50.972	23.951	42.167	1.00 5.28	÷
MOTA	10,67	С	PRO	146	53.863	25.273	43.967	1.00 9.28	÷
ATOM	1068	5	PRO	146	54.272	26.087	43.135	1.00 10.56	3
ATOM	1069	N	GLU	147	54.604	24.825	44.975	1.00 10.54	7
ATOM	1070	CA	GLU	147	55.959	25.281	45.248	1.00 9.65	÷
ATOM	1071	CB	GLU	147	56.894	24.953	44.077	1.00 9.95	Ξ.
ATOM	1072	CC	GLU	147	56.733	23.566	43.456	1.00 18.10	•
ATOM ATOM	1073	CD	GLU	147	57.477	22.401	44.166	1.00 22.76	÷
ATOM	1074 1075		GLU	147 147	58.335 57.207	22.639	45.061	1.00 25.12	Ė
ATOM	1075	C	GLU	147	56.052	21.215 26.773	43.789 45.624	1.00 23.73	÷ ÷
ATOM	1077	5	GLU	147	57.099	27.403	45.453	1.00 10.12	
ATOM	1078	N	THE	148	54.975	27.364	45.124	1.00 10.44	7
ATOM	1079	CA.	THE	148	55.048	29.776	46.541	1.00 10.44	:
ATOM	1080	CB	THE	148	53.778	29.551	45.178	1.00 5.61	•
ATOM	1081		THR.	148	53.589	29.464	44.765	1.00 4.74	3
ATOM	1082	CG:		148	53.881	31.014	45.621	1.00 2.00	÷
ATOM	1083	c	THR	148	55.272	28.818	43.048	1.00 6.00	÷
ATOM	1084	0	THR	148	54.609	28.080	43.789	1.00 4.53	i

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ATOM	1085	N	PRO	149		56.279		605	48.503 47.666	1.00	7.63 4.62		
MOTA	1086	CD	PRO	149		57.156 5 6.62 3		457 757	49.926	1.00	5.20		
MOTA	1087	CA	PRO PRO	149 149		58.074		190	49.860	1.00	2.62		
ATOM	1088	CB CG	PRO	149		58.050		144	48.698	1.00	2.00		
ATOM ATOM	1089 1090	c	PRO	149		55.742		869	50.498	1.00	7.00		
ATOM	1091	ō	PRO	149		55.080		600	49.737	1.00	10.83		
MOTA	1092	Ŋ	MET	150		55.727 54.916		.012 .048	51.814	1.00	5.4		
ATOM	1093	CA	MET	150 150		55.415		.469	52.109	1.00		Š á	
ATOM	1094 1095	CB	MET MET	150		56.864		.812	52.512	1.00		0 :	
ATOM ATOM	1095	SD	MET	150		57.164		.97B	54.292	1.00			
ATOM	1097	CE	MET	150		57.009		.706	54.546 52.169	1.00			
ATOM	1098	С	MET	150		53.411 52.749		.927 .952	52.002	1.00			
MOTA	1099	0	MET THR	150 151		52.878		.696	52.239	1.00	_	-	
ATOM	1100	N CA	THR	151		51.464	30	.405	51.963	1.00			
ATOM ATOM	1102	CB	THR	151		51.157		.902	51.799	1.00			
ATOM	1103	OG	THR	151		51.581		.183	52.955 50.609	1.00			
MOTA	1104		2 THR	151		51.821 50.403		.347	52.922			8	E
ATOM	1105	C	THR THP	151 151		49.218		.919	52.583				-
ATOM	1106 1107	O N	SER	152		50.774		.331	54.123				
MOTA MOTA	1107	CA	SER	152		49.75	3 1	.831	55.041				<u> </u>
MOTA	1109		SER	152		50.178		1.598	56.476	1.0	0 6.4	16	{
ATOM	1110		SER	152		51.02		2.645	56.893			. 7	€ -
ATOM	1111	_	SER	152		49.56		3.321	54.842 55.687				3
MOTA	1112		SER	152		48.98. 50.14		3.976 3.866	53.780				-
ATOM	1113		HIS	153		50.07		5.291	53.48				Ę
ATOM	1114			153 153		51.47		5.883				92	÷
MOTA	1115			153		52.31	-	5.975		6 1.0			ξ
ATOM ATOM	1117		2 HIS	153		52.81	0 3	7.048			_	84	£
ATOM	1116		1 HIS	153		52.78		4.868				02	7
ATOM	1119	CE	1 HIS	153		53.54		5.254			_	19 CO	÷
MOTA	1120		22 HIS	153		53.57		6.570				54	5
MOTA	112		HIS	153		49.27		6.614				78	Ē
MOTA	112		HIS ILE	153 154		48.93		4.38			_	.00	7
MOTA	112 112			154		48.20		34.41		7 1.		.00	÷
MOTA MOTA	112			_		48.49		33.11				.00	÷
ATOM	112		G2 ILE		4	47.90		33.20				.06	*
MOTA	112		G1 ILE			49.9		32.88			-	. SC . OO	÷
ATOM	112		D1 ILE			50.3 46.7		31.72° 34.53				.05	ŧ
ATOM	112					46.1		33.89				.00	:
ATOM						46.0		35.39		35		.56	
MOTA MOTA			A ARC			44.6	38	35.64				.20	•
ATOM	_		B ARC		5	44.3		37.14				.20	5
ATOM	_		G ARC			44.5		37.92			.00 8 .00 14	. 42	÷
ATOM	_		D AR			44.3		39.39			.00 24		-
ATOM			NE AR		55 55	44.2 44.8		41.22		96 1	.00 27	. 35	÷
ATOM		-	CZ AR		55	45.		41.84		99 🗀	.00 25	.45	•
ATOM			NH2 AR		55	44.		41.70			.00 28		:
10ta 10ta			C AR		55	44.		34.9		68 1		5.22	•
ATO			O AR		55	44.1		34.7				5.12 5.08	•
ATO	M 11		N TY		56	42. 42.		34.5				5.24	=
ATO			CA TY		56 56	42.		32.4	-			5.18	-
ATO			CB TY		56 56	42.		31.6		339 :	.00 1	0.55	:
ATO			CG TY		56	43.		31.5		551	00 1	3.49	•
ATO ATO		47	CE1 TY		56	44.	624	30.8			. 00 1		
ATO		48	CD2 TY		56		700	31.0		341 :	1		÷
ATO		49	CE2 TY	(F. 1	.56		895	30.2		646		4.32	:
OTA		150			.56		346	30.2		960 . 380 .	1.00 1 1.00 1	2.25	
ATO		151			56		495 736	29.5 34.6			1.00	7.25	
ATO		152			56		153	35.2		256	1.00	8.18	-
ATC		153			156 157		286	34.5		107	1.00	4.99	
ATC ATC		154 155			157		979	35.0		720	1.00	4.80	:
ATC		156			157	39.	.036	36.2		813	1.00	4.31	
ATC		157	ÇG G	LU :	157		. 632	36.		614	1.::	3.57	
ATO	OM 1	158			157		.577	38.		726	1.00	2.35	
TA		159	OE1 G		157		.568 .486	39. 37.		232 514	1.30	5.11	
ATO		160	OE2 G		157 157		.254	33.		997	1.20	4.09	
TA TA		161			157		799			102	1.00		
W1.			_										

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ATOM	1163	N	VAL	158	37.022	33.675	45.406	1.00 5.40 7
ATOM	1164	CA	VAL	158	36.196		44.842	1.00 6.15
ATOM	1165	CB	VAL	158	35.459	31.877	45.954	1.00 3.03 5
ATOM	1166		VAL	158	34.655	30.759	45.391	1.00 4.03 €
ATOM	1167		VAL	158	36.429		46.962	1.00 3.63 €
ATOM	1168	С	VAL	158	35.154		43.878	1.00 9.07 5
ATOM	1169	0	VAL	158	34.400		44.208	1.00 10.93
ATOM	1170	7.	ASP	159	35.114		42.681	1.00 10.57 7
ATOM	1171	CA	ASP	159	34.147		41.672	1.00 10.09 8
ATOM	1172	CB	ASP	159	34.828		40.327	1.00 11.17
ATOM	1173	CG	ASP	159	33.873		39.256	1.00 13.89
ATOM	1174		ASP	159	33.863		38.172	1.00 13.65
ATOM ATOM	1175		ASP	159	33.093		39.547	1.00 15.65
ATOM	1176 1177	C O	ASP ASP	159	32.997		41.575	1.00 9.91 5
ATOM	1178	N	VAL	159 160	33.227		41.474	1.00 11.09
MOTA	1179	CA	VAL	160	31.766 30.582		41.637	1.00 7.83 7
ATOM	1180	CB	VAL	160	29.637		41.535	1.00 5.49 5
ATOM	1181	CG1		160	28.512		42.755 42.742	1.00 3.19 5
ATOM	1182		VAL	160	30.362		44.091	1.00 3.00 5 1.00 2.00 5
ATOM	1183	c	VAL	160	29.842		40.286	1.00 2.00 5 1.00 6.19 5
ATOM	1184	0	VAL	160	29.364		40.238	1.00 8.22
ATOM	1185	N	SER	161	29.835		39.300	1.00 7.72 7
ATOM	1186	CA	SER	161	29.104		38.046	1.00 8.29 5
ATOM	1187	CB	SER	161	30.094		26.891	1.00 10.26 6
ATOM	1188	OG	SER	161	30.637		26.934	1.00 13.94
ATOM	1189	С	SER	161	28.161	30.275	37.938	1.00 7.24 €
ATOM	1190	0	SER	161	28.601		38.024	
ATOM	1191	N	ALA	162	26.885	30.605	37.791	1.00 7.94 ± 1.00 9.16 T
ATOM	1192	CA	ALA	162	25.793	29.612	27.784	1.00 12.39 5
ATOM	1193	СÐ	ALA	162	24.689		38.736	1.00 15.24 5
ATOM	1194	С	ALA	162	25.199		36.379	1.00 14.12 5
ATOM	1195	0	ALA	162	25.593		35.406	1.00 13.91
ATOM	1196	N	GLY	163	24.220		36.369	1.00 15.85 7
ATOM	1197	CA	GLY	163	23.598		35.150	1.00 16.65
ATOM	1198	С	GLY	163	22.561		34.370	1.00 18.26 6
ATOM	1199	0	GLY	163	21.996		34.897	1.00 18.80 3
ATOM ATOM	1200 1201	N	ASN	164	22.416		33.146	1.00 90.00 7
ATOM	1202	CA CB	ASN ASN	164	21.568		31.994	1.00 90.00 5
ATOM	1203	CG	ASN	164 164	20.505 19.337		31.685	1.00 90.00 5
ATOM	1204		ASN	164	19.322		32.702	1.00 90.00 6
ATOM	1205		ASN	164	18.334		33.726 32.511	1.00 90.00 3 1.00 90.00 7
ATOM	1206	c	ASN	164	20.728		32.186	
ATOM	1207	Š	ASN	164	19.665		32.817	
ATOM	1208	N	GLY	165	21.227		31.601	1.00 90.00 3 1.00 90.00 7
ATOM	1209	CA	GLY	165	20.544		31.514	1.00 90.00 6
ATOM	1210	c	GLY	165	20.274		32.859	1.00 90.00 4
ATOM	1211	0	GLY	165	19.470		32.927	1.00 90.00
ATOM	1212	N	ALA	166	20.941		33.967	1.00 90.00
ATOM	1213	CA	ALA	166	20.602		35.242	1.00 90.00
ATOM	1214	CB	ALA	166	19.550		35.015	1.00 90.00 4
ATOM	1215	С	ALA	166	21.795		36.188	1.00 90.00 5
ATOM	1216	0	ALA	166	21.646		37.421	1.00 90.00 3
ATOM	1217	N	GLY	167	22.964		35.614	1.00 11.62 7
ATOM	1218	CA	GLY	167	24.167	34.185	36.400	1.00 13.44
MOTA	1219	C	GLY	157	24.110	35.688	35.704	1.00 15.68
ATOM	1220	. 0	GLY	167	23.701	36.494	35.863	1.00 15.58 3
ATOM	1221	N	SER	168	24.504	36.099	37.909	1.00 15.58 3 1.00 17.86 7
ATOM	1222	CA	SER	168	24.434		38.252	1.00 18.83 5
ATOM	1223	CB	SER	168	23.543		39.465	1.00 21.81
ATOM	1224	OG	SER	168	22.558		39.118	1.00 23.47
ATOM	1225	C	SER	168	25.820		38.537	1.00 18.61
ATOM	1226	0	SER	168	25.961		38.506	1.00 18.81
ATOM ATOM	1227	;V	VAL	169	26.808		28.789	
ATOM	1228 1229	CA	VA1 VAI	169	28.218		39.149	1.00 17.78
ATOM	1229	CE	VAL	169	28.719		38.657	1.00 19.01 5 1.00 16.57 5
ATOM	1231		VAL	169 169	30.262 28.407		38.769	1.00 16.57
ATOM	1232	002	VAL	169	28.387		37.197	1.00 18.24 5 1.50 17.25 5 1.00 15.44 3 1.00 15.91
ATOM	1233	Ö	VAL	169	28.222		40.666	1.50 17.25
ATOM	1234	N	GLN	170	28.725		41.201	1.00 15.44
ATOM	1235	CA	GLN	170	28.905		42.647	1.00 15.91
ATOM	1236	CE	GLN	170	27.928		43.231	1.00 17.12 5 1.00 19.39 5
ATOM	1237	SC	GLN	170	27.921		44.766	
ATOM	1238	CD	GLN	170	28.202		45.365	1.00 24.35 § 1.00 26.34 §
ATOM	1239	OE1		170	27.369		45.247	
MOTA	1240	NE2	GLN	170	29.33		46.004	1.00 27.24 4 1.00 28.12

ATOM 1241 C GLN	170				
Alon zz-		30.344	36.030		.00 14.76 6
ATOM 1242 0 GLN	170	30.735	34.892		.00 10.49
77.	171	31.101	36.932		00 13.88 7
ATOM 1243 N ARG	171	32.477	36.643		.00 13.53 6
ATOM 1245 CB ARG	171	33.441	37.718		.00 13.16 6
ATOM 1246 CG ARG	171	33.545	37.814		
ATOM 1247 CD ARG	171	34.460	36.758		1.00 13.31 5 1.00 10.48 7
ATOM 1248 NE ARG	171	34.628	36.922		1.00 8.84 5
ATOM 1249 CZ ARG	171	35.274	37.932 38.899	-	1.00 4.37 7
ATOM 1250 NH1 ARG	171	35.841 35.304	38.000		1.00 6.87 7
ATOM 1251 NH2 ARG	171 171	32.581	36.543		1.00 15.23 5
ATOM 1252 C ARG	171	31.706	37.062		1.00 17.57 3
7101.	172	33.651	35.916	46.131	1.00 11.99 7
	172	33.816	35.727	47.565	1.00 9.19 5
A2011	172	33.473	34.260		1.00 10.74 6
ATOM 1256 CB VAL	172	33.300	34.155		1.00 5.41 5
ATOM 1258 CG2 VAL	172	32.236	33.745	47.262	1.00 11.43 6
ATOM 1259 C VAL	172	35.216	35.966	48.031	1.00 9.92 6 1.00 10.28 3
ATOM 1260 O VAL	172	36.134	35.398	47.507	•
ATOM 1261 N GLU	173	35.365	36.778	49.062	1.00 14.35 7 1.00 14.21 5
ATOM 1262 CA GLU	173	36.671	37.041	49.657	1.00 17.07 6
ATOM 1263 CB GLU	173	36.760	38.463	50.218 49.173	1.00 21.96 5
ATOM 1264 CG GLU	173	36.591	39.569 40.903	49.573	1.00 25.14 6
ATOM 1265 CD GLU	173	37.267 37.709	41.647	48.649	1.00 23.21 3
ATOM 1266 OE1 GLU	173	37.709	41.206	50.803	1.00 26.88 3
ATOM 1267 OE2 GLU ATOM 1268 C GLU	173 173	36.910	36.016	50.779	1.00 13.64 5
77.07	173	36.017	35.720	51.592	1.00 13.24 3
7101	174	38.087		50.719	1.00 14.30 7
ATOM 1270 N ILE ATOM 1271 CA ILE	174	38.557	34.406		1.00 14.95 6
ATOM 1272 CB ILE		38.915			1.00 12.11 6
ATOM 1273 CG2 ILE	174	40.014			1.00 13.06 5 1.00 13.75 6
ATOM 1274 CG1 ILE		37.679			1.00 13.75 6 1.00 12.34 6
ATOM 1275 CD1 ILE		36.625			1.00 12.54
ATOM 1276 C ILE		39.802			1.00 17.19 8
ATOM 1277 0 ILE		40.563			1.00 16.67 7
ATOM 1278 N LET		39.982			1.00 16.56 6
ATOM 1279 CA LET		41.138			1.00 15.47 6
ATOM 1280 CB LEG		40.46			1.00 16.91 6
ATOM 1281 CG LEG		40.10			1.00 14.03 6
ATOM 1282 CD1 LET ATOM 1283 CD2 LET		39.34			1.00 16.66 5
		42.39			1.00 16.41 5
7100		42.32		5 53.838	1.00 17.23
ATOM 1285 0 LE ATOM 1286 N GL		43.54	2 35.43		1.00 17.18 7
ATOM 1287 CA GL		44.84			1.00 16.66 6
ATOM 1288 CB GL	176	46.00			1.00 21.33 5
ATOM 1289 CG GL	U 176	45.96			1.00 20.62 6 1.00 22.84 6
ATOM 1290 CD GL		46.14			
ATOM 1291 OE1 G1		47.33			
ATOM 1292 OE2 G1		45.11			
ATOM 1293 C GI		45.06 44.87			
ATOM 1294 0 GI		45.57			_
ATOM 1295 N GI ATOM 1296 CA GI		45.83			1.00 8.11 6
		44.73			1.00 7.43 5
ATOM 1297 C GI ATOM 1298 O GI	_	44.99			2 1.00 9.00 8
ATOM 1299 N A		43.53	34 30.78		
	RG 178	42.3	98 29.8		
	RG 178	41.1			
	RG 178	41.1			
	RG 178	40.9			
	RG 178	41.9			
ATOM 1305 CZ A	RG 178	42.4			5 1.00 26.21 6
ATOM 1306 NH1 A		42.0			
ATOM 1307 NH2 A		43.3 42.3			
	RG 178	42.4			
	RG 178 HF. 179	42.2			
	HF. 179 HR 179	42.1			
	HR 179	43.3			
ATOM 1312 CB 1		43.6	_	03 52.81	8 1.00 12.75
ATOM 1314 CG2 1		44.5	559 27.1	162 51.07	
	HR 179	40.8	373 26.2		
ATOM 1316 0	THR 179	40.1			
	LU 180	39.			
ATOM 1318 CA (SLU 180	38.	469 26.	188 52.16	62 1.00 12.34

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MOTA	1319	СВ	GLU	180	38.329	25.242	53.340	1.00 14.42	5
ATOM	1320	CG	GLU	180	37.418	24.052	53.048	1.00 18.37	ó
ATOM	1321	CD	GLU	180	37.112	23.255	54.299	1.00 19.86	÷
MOTA	1322	OE1	GLU	180	36.526	23.877	55.216	1.00 21.31	3
ATOM	1323	OE2	GLU	180	37.473	22.045	54.387	1.00 18.58	õ
MOTA	1324	C	GLU	180	37.442	27.288	52.301	1.00 14.56	÷
ATOM	1325		GLU	180	37.742	28.385	52.782	1.00 14.76	કે
ATOM	1326	N	CYS	181	36.209	26.986	51.934	1.00 13.B2	7
ATOM	1327	CA	CYS	181	35.149	27.967	52.034	1.00 12.64	5
ATOM	1328	CB	CYS	181	35.382	2 8.9 90	50.936	1.00 12.66	5
MOTA	1329	SG	CYS	181	33.911	29.643	50.288		15
ATOM	1330	С	CYS	181	33.766	27.287	51.905	1.00 13.84	÷
ATOM	1331	0	CYS	181	33.606	26.383	51.086	1.00 15.56	8
ATOM	1332		VAL	182	32.790	27.639	52.743	1.00 13.12	7
MOTA	1333	CA	VAL	182	31.478	26.985	52.613	1.00 11.97	6
ATOM	1334	CB	VAL	182	31.093	26.072	53.820	1.00 9.54	5
ATOM	1335	CG1 CG2		182 182	32.003 29.669	26.307	55.003 54.193	1.00 10.81	6
ATOM	1336 1337	C	VAL	182	30.353	26.255 27.910	52.171	1.00 8.15 1.00 12.84	რ 6
ATOM ATOM	1338	0	VAL	182	29.930	28.828	52.872	1.00 13.90	3
ATOM	1339	N	LEU	183	29.954	27.715	50.930	1.00 11.79	7
ATOM	1340	CA	LEU	183	28.921	28.515	50.338	1.00 12.76	5
ATOM	1341	СВ	LEU	183	29.052	28.500	43.817	1.00 13.26	6
ATOM	1342	CG	LEU	183	30.193	29.380	43.350	1.00 11.81	5
ATOM	1343	CD1		183	30.636	28.956	46.970	1.00 8.24	6
ATOM	1344	CD2		183	29.734	30.852	43.398	1.00 13.01	5
ATOM	1345	c	LEU	183	27.564	28.027	50.778	1.00 14.24	5
ATOM	1346	Õ	LEU	183	27.139	26.887	53.514	1.00 15.09	Š
ATOM	1347	N	SER	184	26.897	28.909	51.487	1.00 14.69	7
ATOM	1348	CA	SER	184	25.583	28.642	51.998	1.00 16.60	έ
ATOM	1349	CB	SER	184	25.558	29.046	53.461	1.00 17.40	6
ATOM	1350	OG	SER	184	26.601	28.369	54.144	1.00 18.79	ā
ATOM	1351	c	SER	184	24.671	29.537	51.208	1.00 17.61	6
ATOM	1352	ō	SER	184	25.115	30.545	53.679	1.00 18.84	3
ATOM	1353	N	ASN	185	23.422	29.140	51.048	1.00 18.50	7
ATOM	1354	CA	ASN	185	22.479	29.998	50.338	1.00 21.04	6
ATOM	1355	СВ	ASN	185	22.463	31.389	51.008	1.00 27.82	6
ATOM	1356	CG	ASN	185	22.274	31.330	52.546	1.00 33.52	6
ATOM	1357	OD1		185	22.899	32.131	53.270	1.00 36.61	3
ATOM	1358		ASN	185	21.392	30.414	53.050	1.00 36.25	7
ATOM	1359	С	ASN	185	22.641	30.149	49.794	1.00 19.48	ó
ATOM	1360	0	ASN	185	22.967	31.228	43.263	1.00 18.46	â
ATOM	1361	N	LEU	186	22.329		43.093	1.00 17.53	7
ATOM	1362	CA	LEU	186	22.384		46.635	1.00 15.82	E
MOTA	1363	CB	LEU	186	23.632		46.201	1.00 14.99	6
ATOM	1364	CG	LEU	136	25.006		45.924	1.00 15.24	5
ATOM	1365	CD1		186	25.951		45.540	1.00 13.51	5
MOTA	1366		LEU	136	25.689	29.663	46.637	1.00 14.02	÷
ATOM	1367	c	LEU	136	21.069		45.261	1.00 16.15	5
ATOM	1368	0	LEU	186	20.449		47.116	1.00 16.68	â
ATOM	1369	N	ARG	187	20.611		45.019	1.00 15.66	7
ATOM	1370	CA	ARG	187	19.371		44.576	1.00 14.27	5
ATOM	1371	СВ	ARG	187	18.845		43.327	1.00 14.63	6
ATOM	1372	CG	ARG	187	19.153		43.263	1.00 19.73	5
ATOM	1373	CD	ARG	187	18.525	30.512	42.054	1.00 23.74	5
ATOM	1374	NE	ARG	187	19.218	30.197	40.905	1.00 26.90	7
ATOM	1375	CZ	ARG	187	18.997	29.109	40.060	1.00 29.07	÷
ATOM	1376	. NH1	ARG	187	18.110		40.430	1.00 29.72	7
ATOM	1377	NH 2	ARG	187	19.594	29.001	33.874	1.00 31.36	7
ATOM	1378	Ç	ARG	187	19.528	26.264	44.298	1.00 16.07	5
ATOM	1379	ာ	ARG	137	20.608	25.788	43.872	1.00 14.20	3
MOTA	1380	N	GLY	138	18.413	25.557	44.483	1.00 15.94	3
MOTA	1381	CA	GLY	188	18.369	24.124	44.291	1.00 17.35	ē
MOTA	1382	C	GLY	188	18.30	23.695	42.842	1.00 19.74	5
ATOM	1383	0	GLY	188	17.76	24.421	42.016	1.00 20.69	=
MOTA	1384	N	ARG	139	18.82	22.492	42.563	1.00 20.12	7
ATOM	1385	CA	ARG	139	18.89	1 21.885	41.239	1.00 20.15	5
ATOM	1386	CB	ARG	189	17.49	5 21.501	41.731	1.00 22.54	5
MOTA	1387	CG	ARG	189	17.45		39.871	1.00 25.04	6
ATOM	1388	CD	AP.G	139	17.78		38.380	1.00 25.92	-5
ATOM	1389	NE	ARG	189	18.57			1.00 27.40	7
MOTA	1390	CZ	ARG	189	18.07			1.00 29.60	4
ATOM	1391		L AF.G	189	16.76			1.00 30.45	;
MOTA	1392		2 ARG	189	18.88			00 29.39	7
ATOM	1393	C	ARG	189	19.61			1.00 20.12	-
ATOM	1394	3	ARG	199	19.40			1.00 21.60	=
ATOM	1395	N	THR	130	20.43			1.00 19.12	7
MOTA	1396	CA	THE	190	21.19	5 24.611	39.812	1.00 17.05	÷

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ATOM	1397 CB	THR	190	2	1.494	25.944	40.460	1.00 15.3	
MOTA		1 THP	190		0.370	26.366	41.226	1.00 18.3	
MOTA		2 THR	190		1.869 2.576	26.984	39.390 39.612	1.00 17.	
ATOM	1400 C	THR	190 190		3.024	23.222	40.428	1.00 17.	12 =
ATOM	1401 O 1402 N	THR ARG	191		3.262	24.460	38.563	1.00 18.	
MOTA MOTA	1403 C		191		4.621	24.01B	38.253	1.00 18.	
ATOM	1404 C	B ARG	191		4.783	23.686	35.746 35.278	1.00 23.	
MOTA	1405 C		191		6.243	23.477 22.032	35.502		
ATOM	1406 CI		191 191		6.824	21.206		1.00 31.	
ATOM ATOM	1407 N		191		7.677	21.329	34.236		
ATOM		H1 ARG	191		28.650	22.261			
ATOM		H2 ARG	191		27.562	20.481			
MOTA	1411 C		191		25.471 25.174	25.213 26.344			
ATOM	1412 O		191 192		26.495	24.950		1.00 12.	
ATOM ATOM		A TYR	192		27.380	25.971	39.901		
ATOM		B TYP			27.283	26.027			
ATOM	1416	G TYR			26.063	26.759			
ATOM	_	D1 TYP			26.105 24.949	28.138			
MOTA		E1 TYP			24.837	26.11			.10 -
ATOM ATOM		CE2 TYP			23.670	26.84			
MOTA		Z TYF			23.745	28.21			
ATOM	1422	OH TYP			22.618	28.97			
ATOM		C TY			28.759 29.134				
ATOM	_	O TYI N THI	_		29.511				.45
MOTA MOTA		CA TH			30.875		0 38.53	_	1.07
ATOM		CB TH			31.036			-	7.66 5 5.74 3
ATOM	1428	OG1 TH			30.030				7.11 6
MOTA		CG2 TH			32.399 31.688				7.05 6
MOTA		C TH			31.370				7.20 3
MOTA MOTA	1431 1432	N PH			32.685			3 1.00	8.39 7
ATOM	1433	CA PH			33.487				5.90 う 6.97 う
MOTA	1434	CB PH			33.421				6.97 5 8.68 5
ATOM	1435	CG PH			32.030				5.87 6
MOTA	1436	CD1 PH	_		31.53				8.15
MOTA MOTA	1437 1438	CD2 PF			30.27				8.14 5
ATOM		CE2 PI			29.95	7 27.4			5.23 á 7.24 á
ATOM	1440	CZ PI			29.48				7.24 5 5.55 5
MOTA		C PI			34.92 35.36		_		5.55 B
ATOM			HE 19 LA 19		35.64				5.34
MOTA MOTA			LA 19		37.05				4.57 :
ATOM			LA 19	5	37.17		_		5.31 6 3.32 6
ATOM			LA 19		37.74				3.32 6 2.79 3
ATOM				95	37.10 39.03		_		2.76 7
ATOM				96 96	39.83				3.78 5
MOTA MOTA				96	40.52		509 43.8		2.00 5
ATO		CG1 V	AL 1	96	40.23				2.00 6 4.04 6
ATON	M 1452	CG2 V		96	40.1				4.54 6 2.07 6
ATO	M 1453			96 96	41.0				5.97
ATO ATO		, О		96 97	41.5			629 1.00	2.00 7
ATO				97	42.6				2.00 5
ATO				97	42.2				
ATO				97	41.3 41.0			574 1.00 504 1.00	2.00
ATO				97 97	40.3			073 1.00	3.47
ATO ATO				97	40.2			517 1.00	2.30
ATO				97	40.8			357 1.00	
ATO		NH2	ARG 1	97	39.7			193 1.00	4.02 2.09
ATC	M 1464			97	43.3	_		362 1.00 280 1.00	3.19
ATC				197 198	42.6 44.7			399 1.00	2.00
ATC ATC				198	45.4			550 1.00	2.47
ATC				198	46.4	420 32		.072 1.00	2.00
ATC	OM 1469	9 C		198	46.3			.442 1.00	5.39
ATC				198	46.			.340 1.00 .612 1.00	
TA				199 199	46. 47.			.694 1.00	
TA TA			ARG	199				.572 1.00	2.00
	OM 147		ARG	199				.270 1.00	5.67

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ATOM	1475	CD	ARG	:99	45.938	40.737	45.915	1.00 9.17	5	
ATOM	1476	NE	ARG	199	46.306		45.579	1.00 13.78	-	
ATOM	1477	CZ	ARG	199	46.187		44.363	1.00 15.94	£	
ATOM	1478	NH1		199	45.738		43.339	1.00 18.32	÷	
ATOM	1479	NH2	ARG	199	46.417		44.181	1.00 18.45	7	
ATOM	1480	С	ARG	:99	48.030		47.023	1.00 5.53	5	
ATOM	1481	0	ARG	199	47.555		48.058	1.00 8.08	į	
ATOM	1482	N	MET	200	49.243		46.984	1.00 5.53	-	
ATOM	1483	CA	MET	200	50.015		48.197	1.00 4.85	5	
ATOM	1484	ĊВ	MET	200	51.484		47.891	1.00 3.73	5	
ATOM	1485	CG	MET	200	52.311		47.346	1.00 4.67	6	
ATOM	1486	SD	MET	200	53.261	36.286	48.538	1.00 9.73	16	
MOTA	1487	CE	MET	200	52.284	34.975	48.812	1.00 2.41	5	
ATOM	1488	C	MET	200	49.340	39.289	48.874	1.00 7.02	5	
ATOM	1489	O	MET	200	49.074		48.228	1.00 6.42	3	
MOTA	1490	N	ALA	201	49.050		50.167	1.00 7.96	7	
ATOM	1491	CA	ALA	201	48.369		50.962	1.00 10.65	5	
ATOM	1492	CB	ALA	201	47.633		52.117	1.00 4.85	6	
ATOM	1493	С	ALA	201	49.261		51.464	1.00 12.36	5	
ATOM	1494	0	ALA	201	50.488		51.453	1.00 13.02	ã	
ATOM	1495	N	GLU	202	48.622		51.901	1.00 15.72	7	
ATOM	1496	CA	GLU	202	49.336		52.421	1.00 19.04	5	
ATOM	1497	CB	GLU	202	48.428		52.276	1.00 23.13	5	
ATOM	1498	CG	GLU	202	47.650		50.914	1.00 28.94	5	
ATOM	1499	CD	GLU	202	48.360		49.757	1.00 31.22	÷	
ATOM	1500	OE1	GLU	202	49.466		49.968	1.00 32.80	3	
ATOM	1501	OE2	GLU	202	47.774		48.634	1.00 30.41	3	
ATOM	1502	ē	GLU	202	49.785		53.903	1.00 19.11	÷	
ATOM	1503	0	GLU	202	49.394		54.561	1.00 20.41	3	
ATOM	1504	N	PRO	203	50.69		54.411	1.00 16.25	7	
ATOM	1505	CD	PRO	203	51.150		55.820	1.00 15.32	5	
ATOM	1506	CA	PRO	203	51.322		53.714	1.00 14.26	5	
ATOM	1507	CB	PRO	203	51.33		54.782	1.00 13.02	6	
ATOM	1508	CG	PRO	203	51.84		55.984	1.00 16.38	5	
ATOM	1509	C	PRO	203	52.740		53.356	1.00 12.03	6	
ATOM	1510	0	PRO	203	53.53		52.985	1.00 15.28	3	
ATOM	1511	N	SER	204	53.07		53.540	1.00 8.98	7	
ATOM	1512	CA	SER	204	54.420		53.222	1.00 11.79	5	
ATOM	1513	CB	SEP.	204	54.674		53.868	1.00 11.87	5	
ATOM	1514	OG	SER	204	55.09		55.224	1.00 12.48	3	
MOTA	1515	C	SER	204	54.68		51.696	1.00 11.88	5	
MOTA	1516	0	SER	204	55.63		51.152	1.00 11.24	5	
ATOM ATOM	1517 1518	N CA	PHE PHE	205 205	53.810 53.90		51.031	1.00 10.89	7	
ATOM	1519	CB	PHE	205	53.91		49.624 49.390	1.00 8.76		
ATOM	1520	CG	PHE	205	55.07		50.052	1.00 8.70		
ATOM	1521		PHE	205	54.85		51.029	1.00 12.81	6	
ATOM	1522		PHE	205	56.38		49.668	1.00 11.00		
ATOM	1523		PHE	235	55.92		51.599	1.00 7.35		
ATOM	1524	CE2		205	57.45		50.237	1.00 11.11		
MOTA	1525	cz	PHE	205	57.21		51.202	1.00 8.98		
ATOM	1526	c	PHE	205	52.74		48.900	1.00 8.87		
ATOM	1527	ō	PHE	295	51.75		49.508	1.00 9.29	_	
ATOM	1528	N	GLY	206	52.91		47.592	1.00 8.57		
ATOM	1529	CA	GLY	206	51.89	2 43.459	46.751	1.00 8.14		
ATOM	1530	С	GLY	206	52.00		45.367	1.00 7.24		
ATOM	1531	0	GLY	206	52.95	6 42.124	45.081	1.00 8.58		
MOTA	1532	. N	GLY	207	51.02	0 43.080	44.520	1.00 7.18		
ATOM	1533	CA	GLY	207	51.12	2 42.534	43.176	1.00 7.59		
ATOM	1534	С	SLY	207	49.82	5 42.355	42.430	1.00 4.80		
ATOM	1535	0	GLY	207	48.85	7 43.048	42.656	1.00 5.05		
ATOM	1536	N	PHE	208	49.78	4 41.332	41.608	1.00 3.71		
MOTA	1537	CA	PHE	208	48.62	1 41.069	40.805	1.00 3.73		
ATOM	1536	CB	PHE	238	49.03	4 41.071	39.322	1.00 6.46		
MOTA	1539	CG	PHE	208	50.15		39.011	1.00 6.53	: :	
ATOM	1540	CD1	PHE	208	49.95		39.004	1.00 6.75	5 5	
ATOM	1541		PHE	208	51.44		38.793	1.00 9.68	3 5	
ATOM	1542		PHE	258	51.02		38.790	1.00 7.99	•	
ATOM	1543		PHE	208	52.50		38.579	1.00 8.12	? 4	
ATOM	1544	CZ	PHE	208	52.29		38.580	1.00 6.95	5 -	
MOTA	1545	С	PHE	208	47.89		41.149	1.00 2.2		
ATOM	1546	0	PHE	208	48.46		41.704	1.00 2.7	7 3	
ATOM	1547	33	TP.P	209	46.60		40.878	1.00 2.30		
MOTA	1548	CA	TP.P	209	45.76		41.073	00 3.7		
ATOM	1549	60	TRP	209	44.30		40.811	1.00 4.7		
MOTA ATOM	1550	CC.	TRP	209	43.50		42.011	1.00 4.7		
ATOM	1551 1552		TP.P	209 209	43.15 42.34		43.104 43.959	1.00 2.6		
	2002	JE	. 45.2	209	42.34	., 59.515	7.7.739	1.00 2.8	7 :	

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	1683	CE3 TI	29	09		43.445	37.	.234	43.446	1.00 2.00 %
MOTA	1553	CD1 T		09		42.908		.586	42.240	1.00 2.25
MOTA	1554			09		42.211		.554	43.396	1.00 2.00 7
ATOM	1555	NE1 T		09		41.825		.309	45.148	1.00 4.70 E
MOTA	1556	CZ2 T		09		42.933		.729	44.616	1.00 4.57 5
ATOM	1557			09		42.131		.513	45.461	1.00 4.76
MOTA	1558			09		46.222		. 604	40.033	1.00 3.17 5
ATOM	1559	-				46.556		. 969	33.920	1.00 3.26 3
ATOM	1560			0.5		46.235		.335	40.412	1.00 4.99
MOTA	1561		_	10				.269	39.533	1.00 5.26 6
MOTA	1562			10		46.650		.002	40.337	1.00 4.60
MOTA	1563		_	10				.363	40.660	1.00 3.40 €
ATOM	1564			110		45.683		. 968	38.515	1.00 9.36 6
ATOM	1565			210		45.571			38.318	1.00 13.86
ATOM	1566			210		44.564		.689 3.924	37.735	1.00 19.41 7
MOTA	1567			211		45.832			36.757	1.00 10.30 6
ATOM	1568			211		44.895		3.423	35.768	1.00 10.37 5
MOTA	1569			211		45.639		2.571	37.567	1.00 11.25 5
ATOM	1570			211		43.893		2.558	38.706	1.00 14.78 3
MOTA	1571			211		44.160		2.175	37.014	1.00 9.47 7
MOTA	1572			212		42.736		2.263	27.734	1.00 7.74 5
ATOM	1573	CA		212		41.791		1.433	36.993	1.00 9.05 5
MOTA	1574	CB		212		40.447		1.434		1.00 4.98 6
ATOM	1575	CG		212		39.723		2.765	35.942	
ATOM	1576	CD2	TRP	212		39.061		3.399	33.030	
ATOM	1577	CE2	TRP	212		38.529		4.597	37.547	
ATOM	1578	CE3	TRP	212		38.867		3.063	39.367	1.00 2.00 5 1.00 2.00 5
ATOM	1579		TRP	212		39.566		3.576	35.867	
MOTA	1580		TRP	212		38.850		4.680	36.219	
MOTA	1581		TRP	212		27.811		5.470	38.359	
ATOM	1582		TRP	212		38.162		3.921	40.167	
MOTA	1583	CH2	TRP	212		37.640		5.111	39.671	
ATOM	1584		TRP	212		42.340		30.012	37.771	•
ATOM	1585	0 6	TRP	212		43.26		29.696	37.043	
ATOM	158		SEF.	213		41.77		29.145		
ATOM	158		SER	213		42.22		27.747		
ATOM	158		SER	213		42.04		27.183		
ATOM			SER	213		40.66	7 :	27.131		
ATOM			SEP.	213		41.30		26.959		
MOTA			SER	213		40.26		27.471		
MOTA			GLU	214		41.64	4	25.718		
ATOM			GLU	214		40.69		24.971		
ATOM			GLU	214		41.30		23.662		
ATOM			GLU	214		42.10		23.79		
ATOM			GLU	214		41.24	19	24.29		
ATOM			GLU	214		41.62	?	25.33		
ATOM			GLU	214		40.21	8	23.63		
ATON			GLU	214		39.55	50	24.81		
ATOL			GLU	214		39.79	23	24.62		
ATON			PRO	215		38.30	01	25.03	7 37.25	8 1.00 11.02 7
			PRO	215		37.95	59	25.36	3 25.80	
ATON		_	PRO	215		37.0		24.96	5 33.0	
ATC!			PRO	215		36.1	55	25.89	6 37.2	90 1.00 9.49 5
OTA OTA			PRO	215		36.4		25.44		
ATO			PRO	21:		36.3		23.60	9 33.2	37 1.00 9.78 🐔
ATO			PRO	215		36.6	64	22.65		
ATO			VAL	21		35.4	4 (°	23.55	3 39.1	
ATO				21		34.6	69	22.34		34 1.00 7.05 🐔
ATO		10 . CB		21		34.7	40	21.82	29 40.9	24 1.00 8.24
ATO			1 VAL	21		35.5	69	20.5		16 1.00 9.46 6
ATO			2 VA1.	21		35.2	226	22.92		
ATO			VAL	21		33.2	61	22.3		
ATC	_	14 0	VAL	21		23.0	001	24.0	39 39.4	
ATC		15 N	SER	21		32.3		21.9	13 39.9	37 1.00 8.47
		16 CA		21		30.9		22.2	47 33.7	
ATC				21		30.5		22.1	57 37.3	c2 1.00 10.83 f
ATO		17 CE		21		29.0		23.1		
ATC				21		30.		21.2		
ATC				21		30.		20.0		347 30 9.60
ATO		520 O		21		29.		21.7		
ATO		521 N		21		28.		20.9		
AT(522 C				28.		21.2		
ATO		523 CI		21	18	27.		20.5		
ATC		524 C				28.		19.1		
AT			D1 LEU		18	28.		21.1		
AT			D2 LEU		1 B		727	21.2		
AT		627 C			18		306			69300 12.22
TA		628 O			18		958			870 1.00 14.15
		629 N			19		486			780 1.00 13.92
AT	OM 1	630 C	A LEU		19	24.				

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bref21c.pdb				Thu	Apr 25	12:27:47	1996		22	
ATOM	1631	СВ	LEU	219	23.86	7 18.372	40.209	1.00	13.95	÷
ATOM	1632	CG	LEU	219	23.81	18.429	23.736		16.57	5
ATOM	1633	CD1	LEU	219	22.85	7 19.303	37.947	1.00	18.05	5
MOTA	1634	CD2	LEU	219	25.208	3 18.410	33.096	1.00	15.67	5
ATOM	1635	С	LEU	219	24.08		42.248	1.00	12.96	÷
ATOM	1636	0	LEU	219	24.37		42.986		12.64	÷
ATOM	1637	N	THP.	220	23.50		42.692		12.52	7
ATOM	1638	CA	THP.	220	23.05		44.068		10.27	÷
ATOM	1639	CB	THP.	220	22.28		44.250	1.00	10.53	÷
ATOM	1640	OG1	THP	220	22.03		42.967	1.00		;
MOTA	1641	CG2	THP.	220	23.07		45.099	1.00	13.55	:
ATOM	1642	0	THR	220	22.11		44.368		11.61	÷
ATOM ATOM	1643 1644	N	THR	220 303	21.190 67.975		43.582		13.03	5
ATOM	1645	CA	THR	303	67.75		64.372	1.00	11.41	7
ATOM	1646	CB	THP.	303	66.40		65.597 66.344		9.49 10.05	é
ATOM	1647	QG1	THE	303	65.98		65.963		12.85	5 3
ATOM	164B	CG2	THF.	303	66.59		67.861		12.80	5
ATOM	1649	c	THR	303	67.73		65.280	1.00	9.93	5
ATOM	1650	ō	THE	303	68.52		65.838	1.00	9.37	3
MOTA	1651	N	TYP	304	66.88		64.343		10.17	7
ATOM	1652	CA	TYP.	304	66.75		63.973	1.00	9.53	ร์
ATOM	1653	CB	TYF.	304	65.30		64.148	1.00	7.06	é
MOTA	1654	CG	TYP.	304	64.83	9 37.937	65.585	1.00	7.97	٤,
MOTA	1655	CD1	TYP	304	64.31	1 39.120	66.072	1.00	4.80	ē.
MOTA	1656	CEl	TYF.	304	64.00.	3 39.268	67.389	1.00	3.80	6
ATOM	1657	CD2	TYF.	304	65.03	0 36.880	66.486	1.00	6.93	÷
MOTA	1658	CE2	TYF.	304	64.72	1 37.015	67.809	1.00	4.43	é
MOTA	1659	CZ	TYP.	304	64.20		68.261	1.00	4.88	÷
ATOM	1660	он	TYP	304	63.88		69.598	1.00	10.24	3
ATOM	1661	C	TYP.	304	67.18		62.554	1.00	8.23	6
ATOM	1662	0	TYP.	304	67.27		61.804	1.00	11.69	5
ATOM	1663	N	SEP.	305	67.47		62.201	1.00	8.34	7
MOTA	1664	CA	SEF	305	67.85		60.843	1.00	9.43	6
ATOM	1665	CB	SEP.	305	69.20		60.838		13.12	5
ATOM	1666	og.	SEP.	305	70.22		61.427	1.00	18.03	8
ATOM	1667	c	SER	305	66.73		60.273	1.00	10.05	6
ATOM ATOM	1668	О М	SER	305	66.49		€0.754	1.00	10.34	ŝ
ATOM	1669 1670	N CA	CYS	306 306	66.09 64.96		59.218	1.00	8.05	7
ATOM	1671	c	CYS	306	64.97		58.619 57.131	1.00	5.52	á
ATOM	1672	0	CYS	306	65.60		56.302	1.00	6.70 6.69	5
ATOM	1673	ED.	CYS	306	63.73		58.889	1.00	6.36	5
ATOM	1674	3G	CYS	306	63.70		60.556	1.00	8.87	15
ATOM	1675	N	HIS	307	64.18		56.808	1.00	6.09	7
ATOM	1676	CA	HIS	307	64.01		55.459	1.00	7.50	ક
ATOM	1677	CB	HIS	307	65.03		55.083	1.00	11.44	ě
MOTA	1678	CG	HIS	307	64.85		55.746	1.30	14.32	5
ATOM	1679	CD2	HIS	307	64.06		55.420	1.00		ج
ATOM	1680	ND1	HIS	307	65.70		55.734	1.00	16.54	7
ATOM	1681	CEI	HIS	307	65.46	7 29.448	55.976	1.00	14.82	5
ATOM	1682	NE2	HIS	307	64.47	8 29.056	56.192		17.24	7
ATOM	1683	C	HIS	307	62.57	6 33.176	55.236	1.00	9.06	÷
ATOM	1684	ο.	HIS	307	61.81	1 32.990	56.188	1.00	11.93	3
MOTA	1685	12	PHE	308	62.16	7 33.136	53.980	1.00	3.50	7
ATOM	1686	CA	PHE	308	60.81		53.647	1.00	5.83	÷
MOTA	1687	CB	PHE	308	50.49		52.167	50	7.92	÷
MOTA	1688		PHE	308	60.53		51.891	1.00	5.48	0.0000000
MOTA	1689		PHE	308	51.14		50.747	1.00		÷
MOTA	1690		PEE	308	59.93		52.73B	1.00		5
MOTA	1691		PHE	308	61.15		50.448	1.00		- 5
ATOM	1692		PHE	308	59.94		52.445	1.00		-
ATOM	1693	22	PHE	308	60.54		51.307	1.00	6.33	- 1
ATOM	1694 1695	÷	PHE	308	60.68		53.849	1.00	5.44	- 1
ATOM ATOM	1695	Ň	PHI Sly	308 309	61.46 59.74		53.322	1.20		1 2
ATOM	1697	o DA	SLY	309	59.51		54.691 54.922	1.00		
ATOM	1698	Ć.	G1.	309	58.31		54.098	1.00	5.83 £ 57	
ATOM	1699	-	SLY	309	57.80		53.316	1.00		2
ATOM	1700	N	PF:	310	57.79		54.233	1.00	5.60	3 ?
ATOM	1701	CD	PP.I	310	58.48		54.742	1.00	9.04	٠.
MOTA	1702	CA	PR.	310	56.64		53.384			6
ATOM	1703	CB	PF.I	310	56.58		53.449	1.00		:
ATOM	1704	CG	PF.I	310	57.95		53.857	1.00		
ATOM	1705	2	PF.C	210	55.39		53.909	1.00		•
ATOM	1706	į.	PRO	310	54.38		53.137	1.00		•
MOTA	1707	2.	LEU	311	55.33	22 28.513	55.161	1.00		
MOTA	1708	CA	LET	311	54.1	45 29.114	55.756	00		÷

bref2	lc.pdb		Thu A	pr 25	12:27:	47 1996	23
ATOM	1709 CB	LEU	311	53.834			1.00 4.94
MOTA	1710 CG	LEU	311	52.83			1.00 5.34 4
ATOM	1711 CD	1 LEU	311	51.524			1.00 5.36 f
MOTA	1712 CD		311	52.684 54.346			1.00 4.95
ATOM	1713 C	LEU	311 311	53.58			1.00 4.76
ATOM	1714 C 1715 N	LEU THP	312	55.39	_		1.00 5.31
MOTA MOTA	1715 N 1716 CA		312	55.68			1.00 7.52 5
ATOM	1717 CB		312	54.77	2 32.7		1.00 7.52
ATOM		1 THR	312	54.89			1.00 10.56 ÷ 1.00 6.36 ÷
ATOM		2 THP.	312	55.11			1.00 6.36 6 1.00 6.58 6
ATOM	1720 0	THR	312	57.16 57.86			1.00 7.15
ATOM	1721 O	THR TRP	312 313	57.64			1.00 5.36
MOTA MOTA	1723 CA		313	59.05		53 58.382	1.00 6.02 6
ATOM	1724 CE		313	59.29			1.00 3.13
MOTA	1725 CC		313	58.93			
MOTA		2 TRP	313	59.68 59.02			
ATOM		E2 TRP E3 TRP	313 313	60.84			
MOTA		D1 TRP	313	57.BE			_
MOTA MOTA		E1 TRP	313	57.93			
MOTA		22 TRP	313	59.48			_
MOTA		23 TRP	313	61.30			
ATOM		H2 TRP	313	60.61 59.60			
MOTA	1734 0	TRP TRP	313 313	58.9			
MOTA MOTA	1735 I 1736 N		314	60.8			7 1.00 .30
MOTA		à VAL	314	61.5			
ATOM		B VAL	314	62.1			
MOTA		G1 VAL	314	62.8			
MOTA		G2 VAL	314 314	61.0 62.6			
ATOM	1741 C		314	63.5			
ATOM ATOM	1742 N		315	62.5		672 61.72	
ATOM		A CYS	315	63.5		567 62.25	
ATOM	1745		315	64.4		948 63.29	
ATOM	1746		315	64.1 62.9		825 63.74 861 6 2.75	
MOTA		B CYS	315 315	62.1		824 61.39	
MOTA MOTA		G CYS	316	65.4		724 63.71	
ATOM		CA LYS	316	66.3	381 33.	242 64.65	0 1.00 9.93
ATOM		CB LYS	316	67.3		320 63.86	
ATOM		CG LYS	316	68.2		.444 64.63 .818 63.70	
ATOM		CD LYS	316 316	69.2 70.2		.818 63.70 .865 63.17	_
MOTA MOTA		CE LYS	316	71.0		.467 €4.28	36004
MOTA		C LYS	316	67.		.462 55.09	2 1.00 10.52
ATOM		D LYS	316	67.		.468 64.3	
MOTA		N PRO	317	67.		.516 65.35 .517 67.4	22 1.00 3.27
ATOM		CD PRO	317 317	67. 68.		.517 67.4° .662 66.8	
ATOM ATOM	1760 1761	CB PRO	317			.412 68.3	and the second s
ATOM		CG PRO	317			.979 68.4	26 1.00 5.27
MOTA		C PRO	317			.714 66.2	
MOTA	1764	1 PRC	317			.732 66.3	
MOTA		N GLN	318			.867 65.7 .137 65.1	
ATOM		CB GLN	318 318			.436 64.3	
ATOM ATOM		CG GLN				.335 62.9	46 1.00 18.24
ATOM		CD GLN				.482 62.0	
ATOM	*.	OE1 GLN				341 61.1	
ATOM		ME2 GLN).642 62.3 7.385 66.3	
ATOM		C GLN				3.237 67.1	
ATOM ATOM		GLN N THR				5.791 55.6	
ATOM		CA THE			.393 30	6.053 54.4	155 1.00 12.38
ATOM		CF THE	403			4.931 54.2	
4OTA	1 1777	OG1 THE				3.658 54.6	
ATON		CG2 THE				4.883 52.° 7.471 54.5	
ATON ATON		C THE				8.341 53.	
OTA		: TY			.778 3	7.694 55.	45 4 1.00 8.68
ATO	M 1782	CA TY	404			9.041 55.	
ATO		CS TY				9.115 55.	
ATO		CG TY				8.968 53. 7.707 53.	
ATO		CE1 TY					042 1.00 2.00
			•				

bref2	lc.po	ib		Thu	Apr	25 1	2:27:4	7 1996		24	
ATOM	1787	CD2	TYR	404	65	.299	40.071	53.050	1.00	2.00	Ę.
ATOM	1788		TYF.	404		. 992	39.918		1.00	2.00	
MOTA	1789	CZ	TYR	404		.709	38.650		1.00	2.53	â
MOTA	1790	ОН	TYR	404	64	.447	38.463		1.00	6.21	
ATOM	1791	С	TYP	404	67	.374	39.373		1.00	6.87	ŧ.
ATOM	1792	0	TYP.	404	67	.459	38.477		1.00	5.71	÷
MOTA	1793	N	SER	405	67	.453	40.653	57.500	1.00	7.44	7
MOTA	1794	CA	SER	405		.581	41.068	58.894	1.00	7.96	ŧ
ATOM	1795	СВ	SEP	405		.842	41.887		1.00	9.81	٤
ATOM	1796	0G	SER	405		. 985	41.082		i.00	14.61	9
ATOM	1797	C	SEF	405		.332	41.863			10.09	÷
ATOM	1798	0	SER	405		.154	43.047			10.03	3
ATOM	1799	N	CYS	406		.466	41.198	60.046		10.45	7
ATOM ATOM	1800 1801	CA C	CYS	406 406		.220	41.789			10.00	
ATOM	1802	0	CYS	406		.192 .900	42.035 41.386			10.98	£
ATOM	1803	СB	CYS	406		.096	40.827			12.25	÷
ATOM	1804	SG	CYS	406		.277	39.951	58.514		12.32	. ć
ATOM	1805	N	HIS	407		.363	42.987			10.98	7
ATOM	1806	CA	HIS	407		.162	43.317		1.00	8.89	5
ATOM	1807	CB	HIS	407	64	.007	44.542			11.52	5
ATOM	1808	CG	HIS	407	63	.779	45.803	63.370		12.77	Ę
ATOM	1809		HIS	407	64	.324	46.233	€2.204	1.00	11.11	÷
MOTA	1810	ND1		407	6.2	.968	46.832	63.B12	1.00	10.97	7
ATOM	1811		HIS	467		.025	47.837		1.00	10.32	÷ -
ATOM	1812	NE 2		407		.840	47.499	61 .9 69	1.00	10.00	-
ATOM	1913	Ç	HIS	407		.687	43.614		1.00	3.26	=
ATOM	1814	0	HIS	407		.078	43.935			10.54	3
ATOM	1815	N	PHE	408		.099	43.443		1.30	7.42	7
MOTA	1816	CA	PHE	408		690	43.746		1.00	6.36	÷
ATOM ATOM	1817 1818	CB CG	PHE	408 408		281	43.636		1.00	5.63	
ATOM	1819		PHE	408		.441	42.280		1.00	3.30	6
ATOM	1820		PHE	408		.411	41.158		1.00	4.11	ž
ATOM	1821		PHE	408		.888	40.882		1.00	4.22 2.80	5 5
MOTA	1822		PHE	408		.626	39.885		1.00	4.80	ě
ATOM	1823	CZ	PHE	408		.866	39.751		1.00	4.71	5
ATOM	1824	С	PHE	408		.459	45.185		1.00	6.02	5
MOTA	1825	0	PHE	408	60	370	46.018	64.744	1.00	8.84	3
ATOM	1826	N	GLY	409	58	3.231	45.463	64.347	1.00	4.91	7
MOTA	1827	CA	GLY	409		7.868	46.791	63.936	1.00	2.33	5
ATOM	1828	c	GLY	409		.494	46.954		1.00	2.02	÷
ATOM	1829	0	SLY	409		.996	46.065		1.00	4.33	÷
ATOM	1830	N	PRO	410		5.879	48.100		1.00	2.00	7
ATOM ATOM	1831 1832	CD CA	PRO PRO	410 410		5.497	49.286		1.00	2.98	÷
ATOM	1833	CB	PRO	410		1.544 1.276	48.397		1.00	3.72	÷
ATOM	1834	CG	PRO	410		5.623	49.754 50.390		1.00	5.67	÷.
ATOM	1835	5	PP.C	410		3.525	47.367		1.00	5.29	
ATOM	1836	ō	PRO	410		2.831	46.752		1.00	7.04 3.58	÷
ATOM	1837	N	LEU	411		3.471	47.165		1.00	6.97	-
ATOM	1838	AD	LEU	411		2.544	46.233		1.00	5.66	•
ATOM	1839	СВ	LEU	411		2.254	46.674		1.00		5
ATOM	1840	CG	LEU	411		1.310	47.803			11.17	÷
ATOM	1841	CD1	LEU	411	50	0.007	47.519			15.07	é
ATOM	1842	CD2	LEU	413		1.888		60.961		14.05	÷
ATOM	1843	С	LEU	411		3.052		62.192	1.00	4.04	-5
MOTA	1844		LEU	411		2.365			1.00	2.7B	-
ATOM	1845	N	THR	412		1.237			1.00		-
ATOM	1846	CA	THE	412		4.749			1.00		5
ATOM ATOM	1847	CE	THR	412		3.985			1.00	2.00	5
MOTA	1848 1849		THR	412 412		4.152			1.00	4.34	•
ATOM	1850	002	THE	412		4.417 6.252			1.00		3
ATOM	1851	ě	THE	412		6.232 6.732			1.00		
ATOM	1852	N	TPP	412		7.003			1.00	3.33	•
ATOM	1853	CA	TRP	413		R.468			1.00		
ATOM	1854	CB	TPP	413		9.003			1.00		
ATOM	1855	CG	TRP	413		8.912			1.00		
ATOM	1856		TEP	413		9.722			1.00		
ATOM	1857		TRP	413		9.374			1.00	3.99	
ATOM	1858		TP.P	413		0.712			1.00		
ATOM	1859		TRP	413		8.121			1.00		
ATOM	1860		TF.P	413		8.395		€1.546	1.00		
MOTA	1861		TRP	413		9.975			1.00	7.15	•
ATOM ATOM	1862		TP.P	413		1.312			1.00		
ATOM	1863 1864	CH2	TRP TEP	413		0.941			50		
772 VI	1004		1 1.5	413	5	8.960	43.72	59.832	:.00	5.50	•

bref21	.c.pdb		Thu	Apr 25	12:2	7:47	1996	25
ATOM	1865	TRF	413	58.187			59.115	1.00 7.06 B
ATOM	1866	VAL	414	60.273			59.813 58.957	1.00 6.50 7 1.00 6.63 5
MOTA		A VAL	414	60.904 61.078			£9.660	1.00 7.88
ATOM		S VAL	414 414	62.19		072	59.029	1.00 6.76 5
MOTA		GI VAL	414	59.78	_	.111	59.547	1.00 3.37 5
ATOM		VAL	414	62.24		.340	58.533	1.00 9.59 5
MOTA MOTA		VAL	414	63.18		.296	59.303	1.00 11.73
ATOM		CYS	415	62.29		.820	57.314	
ATOM		CA CYS	415	63.51		.222	56.809	1.00 9.19 5
MOTA		CYS	415	64.23		.007 .949	55.767 55.189	1.00 8.76
ATOM		CYS	415	63.71 63.20		.882	56.222	1.00 9.11 6
ATOM	_	CB CYS	415 415	62.06		.071	57.341	1.00 14.13 15
MOTA	-	% FAR	416	65.48		.622	55.581	1.00 7.88 7
atom Atom		Ch LYS	416	66.34		.197	5 4.58 5	1.00 3.50 6
ATOM	1881	CB LYS	416	67.17		.349	55.135	1.00 14.71 6
ATOM	1882	CG LYS	416	66.48		.235	56.144	1.00 19.54 5 1.00 23.24 6
ATOM	1883	CD LYS	416	66.61		.629	57.541	1.00 23.24 6 1.00 23.74 6
ATOM	1884	CE LYS	416	65.85		.404	58.599 59.937	1.00 27.08 7
ATOM	1885	NZ LYS	416	66.29		3.888 3.008	54.27B	1.00 12.10 5
MOTA	1886	C LYS	416	67.2: 67.5:		2.187	55.175	
ATOM	1887	C LYS	416 417	67.5		2.817	52.990	1.00 10.95 3 1.00 12.45 7
ATOM	1888	PRO PRO	417	67.2		3.561	51.771	1.00 11.38
ATOM ATOM	1889 1890	CA PRO	417	68.4	34 4	1.684	52.671	1.00 11.76
ATOM	1391	CB PRO	417	€8.3		1.647	51.144	1.30 10.58
ATOM	1892	CG PRO	417	68.2		3.047	50.780	1.00 11.41 6
ATOM	1893	C PRO	417	69.8		1.868	53.221 53.325	1.00 14.43
ATOM	1894	o PRO	417	70.3		2.990 0.762	53.700	1.00 15.69
atom	1895	N GTN	418	70. 4 71.7		0.741	54.209	1.00 16.01 5
MOTA	1896	CA GLN	418 418	71.9		9.562	55.165	_
ATOM	1897	CB GLN	418	71.9		9.963	56.620	1.00 13.51 6
ATOM	1898 1899	CD GLN	418	71.5		8.823	57.530	
MOTA MOTA	1900	OE1 GLN	418	71.3		7.668		
ATOM	1901	NE2 GLN	418	71.4		9.131		
MOTA	1902	C GLN	418	72.0		10.583		
MOTA	1903	0 GLN	418	72.4		39.656		
ATOM	1904	% LYS	510	36.		15.747 44.827		
MOTA	1905	CA LYS	510	36. 37.		45.503		
ATOM	1906	CB LYS	510 510	37.		44.729		9 1.00 24.41 5
ATOM	1907 1908	CO LYS	510	39.		44.786		1 1.00 24.33
ATOM ATOM	1909	CE LYS		40.			3 101.30	
MOTA	1910	NZ LYS				42.90		
MOTA	1911	C LYS				43.642		
ATOM	1912					42.77		·
ATOM	1913	: PHE	_		089 207	42.50		
MOTA	_	CA PHE			903	42.83		
ATOM					969	41.64		2 1.00 17.36
MOTA MOTA					470	40.35		
ATOM	_			30.	594	41.80		5 1.00 19.23
ATOM		CE1 PH	E 51:	•	. 630	39.23		9 1.00 16.04 f 3 1.00 20.47 f
ATOM					.732	40.69		
ATOM					. 271	39.39 41.62		
ATOM				_	.064 .406	40.48		
ATON				-	.416	42.20		72
10ta 10ta				_	.244	41.50		36 1.00 18.20 f
HOTA					.536	42.39	92.1	72 [.00 20.73]
ATO					.498	41.75		
ATO					. 251	40.68		01 1.00 30.11
ATO	M 192				.346	40.50		
OTA					.869	40.0		
ATO		1 0 GI		· -	386.	41.1		
ATO				_	. 984	42.1		30 1.00 13.17
ATO:			ER 51 ER 51	-	9.134	42.0		
ATO ATO			ER 51		9.534	43.3	14 96.4	43 1.00 12.70
OTA				13 40	0.319	43.0		94 1.36 13.07
ATO			ER 5:	13 31	122	40.8		
ATC	M 133	e : s			0.041	40.0		
ATC				-	8.056	40.8		
ATC					7.903 6.839	40.1		
ATC ATC					7.258		65 100.	

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ATOM	1943	CD	LYS	514	36.38	8 41.093	101.842	1.00 2.00	Ξ
ATOM	1944	CE	LYS	514	36.37		102.539	1.00 2.00	į.
ATOM	1945	NZ	LYS	514	35.66		103.798	1.00 3.28	-
ATOM	1946	С	LYS	514	37.62	1 38.443	97. 9 59	1.00 11.50	1
ATOM	1947	0	LYS	514	37.84		98.620	1.00 13.26	÷
ATOM	194B	N	ALA	515	37.13	8 38.401	96.716	1.00 10.50	-
ATOM	1949	CA	ALA	515	36.87		96.038	1.00 9.26	٤
ATOM	1950	CB	ALA	515	36.18		94.719	1.00 10.39	ŧ
ATOM	1951	C	ALA	515	38.16		95.806	ξ3.6 00.1	ē.
ATOM	1952	0	ALA	515	38.17		95.920	1.00 7.Tã	5
ATOM	1953	N	ALA	516	39.24		95.494	1.00 a.76	-
ATOM	1954	CA	ALA	516	40.56		95.204	1.00 7.65	6
ATOM	1955 1956	CB	ALA	516	41.45		94.614	1.00 6.46	5
ATOM ATOM	1957	CO	ALA ALA	516 516	41.20 41.69		96.419 96.353	1.00 7.97	÷.
ATOM	1958	N	LEU	517	41.22		97.530	1.00 8.85 1.00 8.04	ė 7
ATOM	1959	CA	LEU	517	41.80		98.743	1.00 5.52	ś
ATOM	1960	СВ	LEU	517	41.44		99.947	1.00 3.15	-6
ATOM	1961	CG	LEU	517	42.14		100.158	1.00 4.53	Ę
ATOM	1962		LEU	517	41.71		99.108	1.00 9.66	5
ATOM	1963		LEU	517	41.75		101.519	1.00 4.29	5
ATOM	1964	С	LEU	517	41.27		98.992	1.00 7.39	ē
ATOM	1965	0	LEU	517	42.00	9 33.751	99.437	1.00 10.93	=
ATOM	1966	N	LEU	518	39.99	7 34.433	93.648	1.00 3.49	7
ATOM	1967	CA	LEU	518	39.29	33.177	98.857	1.00 7.25	÷
ATOM	1968	CB	LEU	518	37.84		99.273	1.00 5.35	ŧ
MOTA	1969	CG	LEU	518	37.61	4 33.731	100.773	1.00 5.58	5
ATOM	1970	CD1	LEU	518	36.80	34.965	100.936	1.00 3.48	5.
ATOM	1971		LEU	518	36.95		101.495	1.00 6.87	5
ATOM	1972	C	LEU	518	39.33		97.733	1.00 9.11	5
ATOM	1973	0	LEU	518	39.18		97. 9 79	1.00 8.10	3
ATOM	1974	Ŋ	ALA	519	39.55		96.505	1.00 11.23	7
ATOM	1975	CA	ALA	519	39.60		95.342	1.00 13.55	5
ATOM	1976	СВ	ALA	519	39.31		94.072	1.00 12.74	5
ATOM	1977	C	ALA	519	40.90		95.209	1.00 15.14	6
ATOM	1978	0	ALA	519	41.73		94.311	1.00 15.55	Ξ
ATOM	1979	N	ALA	520	41.04		96.068	1.00 17.93	7
ATOM ATOM	1980 1981	CA CB	ALA ALA	520 520	42.22		96.115	1.00 19.81	é
MOTA	1982	C	ALA	520	42.1		97.371 94.865	1.00 20.83	Ę
ATOM	1983	0	ALA	520	41.7		94.339	1.00 19.39	÷
ATOM	1984	N	ARG	521	43.83		94.449	1.00 90.00	7
ATOM	1985	CA	ARG	521	44.40		93.322	1.00 90.00	
ATOM	1986	CВ	ARG	521	45.4		92.652	1.00 90.00	5
ATOM	1987	CG	ARG	521	45.1		92.441	1.00 90.00	÷
ATOM	1988	CD	ARG	521	45.75		93.500	1.00 90.00	÷
ATOM	1989	NE	ARG	521	45.5		94.854	1.00 92.00	-
MOTA	1990	CZ	AP.G	521	46.2	79 29.452	95.464	1.00 93.33	•
ATOM	1991	NH1	ARG	521	47.3	51 28.95?	94.843	1.00 90.00	-,
ATOM	1992	NH2	ARG	521	45.8	86 28. 88 9	96.620	1.00 90.00	-
MOTA	1993	C	ARG	521	45.0	18 26.343	93.866	1.00 90.00	÷
ATOM	1994	0	ARG	521	44.8		95.032	1.00 90.00	Ē -
ATOM	1995	ĸ	GLY	522	45.7		93.022	1.00 90.00	
ATOM	1996	CA	GLY	522	46.3		93.500	1.00 93.30	ŧ
MOTA	1997	č	GLY	522	47.8		93.549	1.00 90.00	÷
ATOM	1998	Č.	GLY	522	48.2		93.891	1.00 90.00	3
ATOM	1999	. CD	PRO	523	18.6		93.225	2.00 95.00	
MOTA MOTA	2000	. CD	PRO	523	48.0			1.00 90.00	÷
MOTA	2001 2002	CA	PRO PRO	523 523	50.1 50.4			1.00 90.00	5
ATOM	2002	CG	PRO	523	49.2			1.00 90.00	÷
ATOM	2004	5	PRO	523	50.9			1.00 90.00	
ATOM	2005	Š	PRO	523	50.4			1.00 93.30	
ATOM	2006	N	SLU	524	52.2			1.00 93.30	-
ATOM	2007	CA	GLU	524	53.1			00 23.63	•
ATOM	2009	40	GLU	524	54.2			1.00 27.67	:
ATOM	2009	cs	GLU	524	55.4			1.00 23.39	:
ATOM	2010	ÇD	GLU	524	55.2			1.00 23.39	<u> </u>
ATOM	2011		GLU	524	54.9			1.00 23.10	÷
ATOM	2012		GLU	524	55.3			1.00 30.26	•
ATOM	2013	c	GLU	524	53.6			1.00 21.32	- 4
ATOM	2014	€.	GLU	524	53.7			1.00 25.22	:
ATOM	2015	N	GLU	5.25	54.1			1.00 16.30	
ATOM	2016	CA	GLU	525	54.7			1.00 13.58	;
MOTA	2017	CE	GLU	525	53.5			1.00 18.50	•
ATOM	2018	CG	GLU	525	53.E			1.00 27.12	;
ATOM	2019	CD	GLU	521	52.5				5
ATOM	2020	OE:	I GLU	525	52.4	174 23.956	85.991	1.00 33.25	i

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	2021 0	E2 GLU	525	51.731	26.066		.00 34.53
ATOM ATOM	2022 C		525	55.572	27.633		.50 8.91 = 1.00 9.70 = 1.00
ATOM	2023 0		525	55.306	28.676 27.495		.30 5.52
MOTA	2024 N		526 526	56.619 57.455	28.638		1.00 4.14
MOTA	2025 C		526 526	58.859	28.182		1.00 4.80 E
MOTA		B LEU G LEU	526	60.103	29.082		1.00 2.00
ATOM ATOM		D1 LEU	526	61.166	28.507		1.00 2.00 £
ATOM	2029 C	D2 LEU	526	59.856	30.499		1.00 2.00 5
MOTA	2030		526	56.688 56.527	29.248 28.607		co 2.ao :
MOTA	2031		526 527	56.209	30.474		1.00 2.00
MOTA	2032 N 2033 C	CA LEU	527	55.415	31.107	85.954	1.00 2.00
MOTA MOTA		B LEU	527	54.115	31.638	86.441	1.00 4.05 f
ATOM	2035	CG LEU	527	53.035	30.653	86.824	1.00 2.65 f
ATOM		CD1 LEU	527	51.951 52.547	31.429 29.889	87.441 85.620	1.00 2.00
MOTA		CD2 LEU	527 527	56.110	32.256	85.176	1.00 4.04
ATOM		C LEU	527	56.413	33.252	85.836	1.00 5.30
MOTA MOTA		N CYS	528	56.234	32.176	83.844	1.00 3.62
MOTA		CA CYS	528	56.929	33.199	83.051 82.044	1.00 2.97 1 1.00 2.18
MOTA		C CYS	528	55.987 55.087	33.810 33.127	81.560	1.00 2.61
MOTA	-	O CYS	528 528	58.132	32.593	62.282	1.00 2.00 1
MOTA MOTA	2044 2045	SG CYS	528	59.491	31.832	83.234	1.00 2.00 15
MOTA	2046	N PHE	529	56.197	35.088	61.743	1.00 2.00 T
MOTA	2047	CA PHE	529	55.397	35.792	80.75B 81.303	1.00 4.1 6 f
MOTA	2048	CB PHE	529	54.008 53.980	36.143 37.315	82.231	1.00 2.00
ATOM	2049	CG PHE	529 529	53.958		81.733	1.00 2.00
ATOM	2050 2051	CD1 PHE	529	53.912			1.00 2.00
MOTA MOTA	2051	CE1 PHE	529	53.868			1.00 2.00
MOTA	2053	CE2 PHE		53.822			1.00 2.00 1 1.00 2.00 1
ATOM	2054	CZ PHE		53.801			1.00 5.77
ATOM	2055	C PHE		56.100 57.078			
ATOM	2056 2057	O PHE		55.665			1.00 6.52 1.00 2.84 1.00 2.00 f
ATOM ATOM	2058	CA THE		56.225	38.655		
MOTA		CB THE		57.228			1.00 2.00 f 1.00 2.64 f
ATOM		OG1 THE		57.683			1.00 2.64 : 1.00 2.96 :
atom		CG2 TH		56.63° 55.07°			
ATOM		C THE		53.99			
ATOM ATOM		N GLI		55.27	5 40.88		1.00 2.23
ATOM		CA GL	j 531	54.24			
ATOM		CB GL		54.17 54.04			
ATOM		CG GL		53.77			1.00 14.12
ATOM		OE1 GL		54.08			1.00 15.54
10TA 10TA		OE2 GL		53.22			
ATON		C GL	ປ 531	54.46			
MOTA	-			53.50 55.65			
ATO				56.03			2 1.00 6.83
ATOI ATOI				56.90	0 44.79		
OTA			RG 532				4 1.00 4.16 E 3 1.00 6.94 E
ATO	M 2077						_
ATO			RG 532 RG 532				0 1.00 17.72
ATO ATO						96 73.97	
OTA			RG 532				/ 13.00
ATO	M 2082	C A	RG 532				
ATC			RG 532				
ATC			EU 533 EU 533				5 1.00 12.12
ATC ATC			EU 531			90 71.82	1 1.00 13.13
ATC			EU 53:	56.8	84 40.2	98 71.74	1 1.00 10.95
ATC		e odi 1	EU 53:	56.5			
ATO	M 208	9 CD2 L					
ATO			.EU 53				
ATC		_	.EU 53				6600 12.95
TA TA			EC 53	_	722 42.5	523 75.0	
AT			:LU 53	4 61.4			6500 16.94
AT	OM 209	5 CG (3LU 53				
AT			310 53 310 53				
TA TA	OM 209						

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ATOM	2099	С	GLU	534	61.	892	42.579	75.527	1.00	10.95	÷
ATOM	2100	C	GLU	534		651	43.380	77.066		10.92	
ATOM	2101	N	ASP	535	61.	251	41.637	77.194	1.00	9.01	;
ATOM	2102	CA	ASP	535		247	41.578	78.638	1.00	6.92	₹.
ATOM	2103	CB	ASP	535		188	42.544	79.128	1.00	8.31	÷
ATOM	2104	CG	ASP	535		848	42.334	78.430	1.00	8.75	ŧ
ATOM ATOM	2105 2106		ASP	535		020	41.541	78.913	1.00	11.89	3
ATOM	2100	002	ASP ASP	535° 535		635 793	42.949	77.372	1.00	15.77	5
ATOM	2108	Ö	ASP	535		063	40.201 39.577	79.033 73.295	1.00	6.27	5
ATOM	2109	N	LEU	536		178	39.731	80.204	1.00	6.65 5.28	7
ATOM	2110	CA	LEU	536		717	38.436	80.651	1.00	4.48	é
ATOM	2111	CB	LEU	536		614	37.315	80.149	1.00	2.00	÷
ATOM	2112	CG	LEU	536	61.	012	35.958	80.495	1.00	2.00	5
ATOM	2113	CD1	LEU	536	59.	697	35.789	79.782	1.00	2.00	Ę
ATOM	2114		LEU	536		955	34.853	80.152	1.00	2.00	ó
ATOM	2115	Ċ	LEU	536		725	38.468	82.154	1.00	5.42	é
ATOM	2116	0	LEU	536		701	38.896	82.751	1.00	5.81	3
ATOM ATOM	2117 2118	N CA	VAL VAL	537 537		60€ 514	38.093	82.767	1.00	6.59	7
ATOM	2119	CB	VAL	537		514 439	38.050 39.006	84.219	1.00	4.71	6
ATOM	2120	CG1		537		391	38.900	84.761 86.262	1.00	3.90	5
MOTA	2121		VAL	537		754	40.434	E4.386	1.00	7.66 6.66	-5 -5
ATOM	2122	c	VAL	537		111	36.652	84.604	1.00	2.70	÷
ATOM	2123	0	VAL	537		232	36.096	83.977	1.00	5.62	à
MOTA	2124	N	CYS	538	59.	812	36.048	85.553	1.00	3.31	7
ATOM	2125	CA	CYS	538	59.	452	34.711	65.055	1.00	4.73	5
ATOM	2126	C	CYS	538		375	34.771	87.597	1.30	5.86	5
ATOM	2127	0	CYS	538		165	35.457	63.257	1.00	6.30	Ξ
MOTA	2128	CB	CYS	538		438	33.619	85.600	1.50	2.00	ē
ATOM ATOM	2129 2130	SG N	CYS PHE	538 539		634 426	33.421	83.795	1.00	3.79	15
ATOM	2131	CA	PHE	539		267	34.059 34.099	88.178 89.621	1.00	3.78	7
ATOM	2132	CB	PHE	539		295	35.232	89.997	1.00	4.15 4.88	5 5
MOTA	2133	CG	PHE	539		852	35.009	89.515	1.00	7.86	5
ATOM	2134		PHE	539		835	34.690	90.420	1.00	5.60	6
ATOM	2135		PHE	539		519	35.104	88.147	1.00	9.65	é
MOTA	2136	CE1	PHE	539	53.	540	34.470	89.986	1.00	4.81	á
ATOM	2137		PHE	539	54.	201	34.878	87.706	1.00	7.22	5
ATOM	2138	CZ	PHE	539		223	34.562	88.630	1.00	5.52	ć.
ATOM	2139	С	PHE	539		689	32.807	90.123	1.00	3.30	÷
ATOM	2140	0	PHE	539		397	31.913	89.352	1.00	5.07	.3
ATOM ATOM	2141 2142	N CA	TF.P	540		606	32.696	91.436	1.00	2.62	7
ATOM	2143	CB	TRP TRP	540 540		965 859	31.575	92.102	1.00	5.41	5
ATOM	2144	CG	TRP	540		890	30.380	92.252 93.315	1.00	5.13 7.06	é
ATOM	2145	CD2		540		250	30.807	93.175	1.50	4.64	÷ ÷
ATOM	2146	CE2		540		861	30.657	94.430	1.50	5.73	÷
ATOM	2147	CE3	TP.P	540	61.	800	31.299	92.110	1.00	5.86	5
ATOM	2148	CD1	TRP	540	58.	738	29.995	94.610	1.56	8.29	é
ATOM	2149	NE 1		540		914	30.161	95.286	1.00	8.36	7
ATOM	2150	CZ2	TRP	540	62.	208	30.984	94.657	1.00	8.15	÷
ATOM	2151		TRP	540		336	31.623	92.328	1.00	7.58	÷
ATOM ATOM	2152 21 5 3		TRP	540		927	31.465	93.596	1.00	8.06	÷
ATOM	2154	O O	TRP TRP	540 540		504 774	32.189 33.366	93.417 93.668	1.00	6.24	é
ATOM	2155	19	GLU	541		698	31.467	94.186	1.00	7.32 8.81	.3
ATOM	2156	· CA	GLU	541		187	31.399	95.452	1.00	10.45	7
ATOM	2157	CB	GLU	541		768	32.565	95.270		11.89	÷
MOTA	2158	CG	GLU	541		592	33.523	94.070		14.89	5
MOTA	2,59	CD	GLU	541	52.	202	34.134	93.991		16.24	
ATOM	2160		GLU	541	52.	. O94	35.229	93.415		17.33	à
ATOM	2161		GLU	541		.219	33.550	94.516	1.00	16.64	.3
ATOM	2162	Ç	GLU	541		148	30.925	95.507		10.03	-5
atom atom	21.53	O	GLU	541		. 744	29.811	95.232	1.00	10.32	3
ATOM	2164 2165	CA	GLU	542 542		.552 .521	31.242	97.724	1.00	10.91	•
ATOM	2166	CB	GLU	542		.321	30.222 29.482	98.766 98. 8 33	00	10.78 10.24	5
ATOM	2167	CG	GLU	542		.122	30.359			14.40	-5
ATOM	2168	CD	SLU	542		.400	29.571	99.006		15.97	•• ••
MOTA	2169		GLU	542		711		100.188	1.00	17.03	3
ATOM	2170	OE2	GLU	542		.095	29.263	98.026	1.00	17.30	3
ATOM	2171	0	GLU	542		.083		100.128	1.00	9.66	•
ATOM	2172		GLU	542		.741		100.248	1.00	9.88	. ;
ATOM	2173	33	ALA	543		. 051		101.135	1.00	6.81	••
atom atom	2174 2175	GA GD	ALA	543		. 652		102.493	1.50	7.10	-5
ATOM	2176	C	ALA ALA	543 543		.466 .716		103.325	1.00	4.26	÷
		_			32	0	51.141	10.7.108	1.00	8.56	·š

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MOTA	2177	0 1	ALA	543	56.91			102.998		10.8	3 E	
MOTA			ALA	544	55.28			103.695	1.00	9.4 0 10.4		
MOTA	2179	CA I	ALA	544	56.19			104.325		0 11.5		
ATOM	2180		ALA	544	55.42			104.890 105.438		0 11.8		
MOTA	2181	-	ALA	544	56.80 56.1			106.216		0 13.6		
MOTA	2182		ALA	544 545	58.2			105.456		0 12.1		
MOTA	2183		SER SER	545	58.9			106.453	1.0	0 13.0	8 6	
MOTA	2184 2185	CA CB	SER	545	59.3			105.980	1.0	0 12.9		
ATOM ATOM	2186	OG	SER	545	€0.2	91 2		106.827		0 14.0	26	
MOTA	2187	C	SEP.	545	60.2			106.891		0 14-0		
ATOM	2188	С	SER	545	60.8			106.117		0 15.		-
MOTA	2189	N	ALA	546	60.5			108.174		0 17.	-	
MOTA	2190	CA	ALA	546	61.6 61.9			110.200		0 17.		Ē
ATOM	2191	СВ	ALA ALA	546 546	62.9			108.143		00 18.	94	£
MOTA	2192	C O	ALA	546	63.6			107.75		00 19.	69	5 -
ATOM	2193 2194	N	GLY	547	63.2			107.96	5 1.0	00 19.		
ATOM ATOM	2195	CA	GLY	547	64.4	38 3		107.30		00 20.		é
ATOM	2196	c	GLY	547	64.6			106.03		00 20.		ક
ATOM	2197	Ç	GLY	547	66.0			105.73		00 23.		5
ATOM	2198	N	VAL	548	63.1			105.32		00 18. 00 14.		Ę
MOTA	2199	CA	VAL	548	64.			104.04		00 14.		ŧ
ATOM	2200	CB	VAL	54B	63.			102.36	3	00 13.	62	ē
MOTA	2201		VAL	548	63. 63.			104.75		00 11.	28	ŧ
MOTA	2202		VAL VAL	548 548	63.			102.99		00 15.	. 33	5
ATOM	2203 2204	00	VAL	548	62.	721	34.309	102.71	4 :.	00 16.	.13	3
ATOM ATOM	2205	N	GLY	549	64.	954	34.612	102.54		00 15		-
ATOM	2206	CA	GLY	549			35.667		1 1.	00 12	. 34	ē
ATOM	2207	С	GLY	549				100.26		00 12	.73	á E
ATOM	2208	0	GLY	549			33.991			00 11		7
MOTA	2209	И	PRO	550			36.066 37.459			00 12		5
ATOM	2210	CD	PRO	550 550		213 271	35.63			00 13		5
ATOM	2211	CA CB	PRO PRO	550		333	36.94				.83	ક
MOTA	2212 2213		PRO	550		201	38.01		99 1.	.00 10	.09	÷
MOTA MOTA	2213		PRO	550		647	34.96			.00 13		÷
ATOM	2215		PRO	550		991	34.06			.00 14		3
ATOM	2216		GLY	551		384	35.34			.00 13		7
ATOM	2217		GLY	551		714	34.79			.00 11	.00	÷
MOTA	2218	C	GLY	551		.776	33.30			.00 9		-
MOTA	2219		GLY	551		. 854	32.73	-			5.84	÷
MOTA	2220		ASN	552		.625 .573	31.21				5.10	5
ATOM	2221			552 552		.510		1 100.9			1.08	÷
ATOM	2222					.797	31.44		26 :		6.03	:
MOTA MOTA	222		1 ASN			.789		2 102.8			7.24	3
ATOM	222		2 ASN			.991		1 102.€			3.39	
ATOM			ASN	552		.287	30.50				7.54	5 3
ATOM		7 0	ASN			.176	29.26				7.91 5.28	7
ATOM			TYR			.157	31.2				4.43	÷
ATOM						.867	30.73				4.87	÷
ATOM						.367	30.3		520	00	4.46	Æ
ATOM			D1 TYF			1.491	31.0		373 :	1.00	3.71	٤
ATOM ATOM			E1 TYF			3.574	30.2	90 93.	117	1.00	3.40	:
ATOM			D2 TYP			5.280	28.9		423	1.00	3.40	5
ATOM			E2 TYF	5.5		1.355	28.2		167	1.00	3.44	÷
ATOM						3.516	28.9		012		2.00	:
ATON	1 223				-	2.650	28.1		110	1.00	3.67 5.08	
MOTA						8.791	31.2 32.3			1.00	4.35	:
CTA					-	9.432 8.845	30.5		980	1.30	5.81	-
OTA						9.622	31.1		363	1.50	5.70	:
ATO			A SE			0.999			332	1.00	3.42	:
ATO			G SE		-	0.954			214	1.00	11.53	÷
ATO! ATO!						8.800			621	1.00	5.93	:
OTA					-	8.289	29.	584 91.	502	1.00	7.83	- 3
ATO			PH	E 55	55 6	8.574			773	1.00	5.48	
ATO	M 22	47 (A PH			7.811			536	1.00	5.32 5.75	
OTA			D PH			6.734			. 484 . 335	1.00	5.98	
ATO			CG PH			55.780 54.423			.567	1.00	3.96	
ATO			DD1 PH			6.242			.319	1.00	4.43	
OTA OTA			CE1 PH			53.541		_	.507	30	5.29	
ATC			CE2 PF		5.5	55.379	32.	427 85	. 963	1.00	3.92	
ATC			CZ Pł		55	64.030	32.	339 86	.196	1.00	5.62	

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ATOM	2255	С	PHE	555	68.77	9 31.759	88.337	1.00	6.86	÷
MOTA	2256	0	PHE	555	69.18		87.945	1.00	8.43	3
ATOM	2257	N	SER	556	69.09		£7.740	1.00	7.22	7
ATOM	2258	CA	SER	556	70.01	9 30.503	86.619	1.00	6.83	÷
ATOM	2259	CB	SER	556	70.96	9 29.315	86.879	1.00	4.30	ó
ATOM	2260	OG	SER	556	71.92	3 29.587	87.891	1.00	8.78	3
ATOM	2261	С	SER	556	69.33	6 30.298	85.257	1.00	5.62	÷
ATOM	2262	0	SER	556	68.53	5 29.389	85.117	1.00	8.35	=
ATOM	2263	N	TYR	557	69.68	2 31.102	84.255	1.00	3.08	7
ATOM	2264	CA	TYP.	557	69.12	30.943	82.924	1.00	3.30	÷
ATOM	2265	CB	TYP.	557	68.19	8 32.089	82.569	1.00	2.00	Ę.
ATOM	2266	CG	TYP	557	68.83	2 33.434	82.422	1.00	2.00	÷
ATOM	2267	CD1	TYP.	557	69.40	5 33.825	81.218	1.00	2.00	é
ATOM	2268	CE1	TYF.	557	69.85		€1.023	1.00	2.56	÷
MOTA	2269	CD2	TYR	557	68.73		83.434	1.00	2.00	5
MOTA	2270	CE2	TYR	557	69.18		83.260	1.00	2.00	÷
ATOM	2271	cz	TYR	557	69.73		82.051	1.00	3.10	5
MOTA	2272	ОН	TYR	557	70.12		81.865	1.00	3.23	9
ATOM	2273	C	TYR	557	70.19		81.870	1.00	3.33	÷
ATOM	2274	0	TYR	557	71.31		B2.090	1.00	4.25	3
ATOM	2275	N	GLN	558	69.83		80.695	1.00	3.52	7
ATOM	2276	CA	GLN	558	70.83		79.648	1.00	3.20	5
ATOM	2277	CB	GLN	55B	71.60		79.828	1.00	3.66	÷
ATOM	2278	CG	GLN	558	72.50		78.648	1.00	6.55	÷
ATOM	2279	CD	GLN	558	73.17		73.788	1.00	5.14	÷
ATOM	2280		GLN	558	72.55	_	79.183	1.00	6.68	3
ATOM	2281		GLN	558	74.44		78.477	1.00	7.23	7
MOTA	2282	C	GLN	558	70.20		73.279	1.00	3.24	ź
ATOM	2283	0	GLN	558	69.42		77.977	1.00	2.96	3
ATOM	2284	N	LEU	559	70.51		77.445	1.00	2.00	7
MOTA	2285	CA	LEU	559	69.94		76.120	1.00	2.89	÷
ATOM	2286	CB	LEU	559	70.03		75.399	1.00	2.00	÷
MOTA	2287	CG	LEU	559	68.97		75.792	1.00	2.00	6
ATOM	2288		LEU	559	69.10		75.005	1.00	2.00	÷
ATOM	2289		LEU	559	67.63		75.564	1.00	2.00	5
MOTA	2290	С	LEU	559	70.7		75.447	1.00	5.30	5
MOTA	2291	0	LEU	559	71.9		75 .728	1.00	4.67	3
ATOM	2292	N	GLU	560	70.09		74.718	1.00	6.97	7
ATOM	2293	CA	GLU	560	70.7		7 3.997	1.00	11.03	5
ATOM	2294	CB	GLU	560	69.78		72.938	1.00	14.40	÷
MOTA	2295	CG	GLU	560	70.2		72.163		19.08	ó
MOTA	2296	CD	GLU	560	69.70		70. 7 38	1.00		÷
ATOM	2297	OE1		560	69.7		69.983		25.39	3
MOTA	2298		GLU	560	69.20		70.346	1.00	21.83	æ
ATOM	2299	C	GLU	560	71.9		73.310		11.71	ર્ગ
ATOM	2300	0	GLU	560	71.9		72.505	1.00	10.88	3
ATOM	2301	N	ASP	561	73.1		73.648	1.00	12.36	-
ATOM	2302	CA	ASP	561	74.4		73.118	1.00	13.20	5
ATOM	2303	CB	ASP	561	74.4		71.589	1.00	11.29	ć
ATOM	2304	CG	ASP	561	74.4		70. 96 8	1.00	13.29	÷
ATOM	2305		ASP	561	74.5		71.725		14.53	ê
ATOM	2306	OD2	ASP	561	74.2	96 26.963	69.729	1.30	11.84	Ξ
MOTA	2307	С	ASP	561	74.9		73.661	1.00	17.27	÷
ATOM	2308	0	ASP	561	75.6		72.931		21.27	3
ATOM	2309	N	GLU	562	74.7		74.926		17.40	7
ATOM	2310	CA	GLU	562	75.2		75.504		16.45	40 40 40 40 40 40 40 40 40 40 40 40 40 4
MOTA	2311	CB	GLU	562	74.0		75.652		20.22	÷
ATOM	2312	' CG	GLU	562	73.2		74.408	1.00	23.17	ć
MOTA	2313	CD	GLU	562	73.9		73.289		23.82	÷
ATOM	2314		GLU	562	74.3		73.511		22.18	3
ATOM	2315		GLU	562	73.9		72.169	1.00	27.47	3
MOTA	2316	0	GLU	562	75.7		75.871		14.28	÷
MOTA	2317	0	GLU	562	75.4				15.04	÷
ATOM	2318	N	PRO	563	76.6		77.465	1.00	11.29	:
ATOM	2319	CD	PRI	563	77.2		77.064	1.53		:
ATOM	2320	CA	PRC	563	77.1		73.794	1.00	11.69	
ATOM	2321	CP	PRC	563	78.1			1.00	7.10	
MOTA	2322	CG	PRC	563	77.6			1.00	5.79	
ATOM	2323	C	PRC	563	75.9			1.00	10.73	÷
ATOM	2324	0	PRC	563	74.9		79.558	1.20	11.56	:
ATOM	2325	N	TEP	564	75.9			1.00	8.20	
ATOM	2326	CA	TPP	564	74.9			1.00	5.30	
ATOM	2327	40	TP.F	564	75.3			1.00		•
ATOM	2328	CG	TRP	564	74.6			1.00	5.38	•
ATOM	2329		TRF	564	73.2			1.20	5.62	5
ATOM	2330		TRF	564	73.1			00		5
ATOM	2331		TRP	564	72.1			1.00		;
ATOM	2332	CD:	TP.F	564	75.2	25C 26.700	82.387	1.50	5.26	÷

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ATOM	2333	NE 1	TRP	564	7	4.33	8 3	25.	675	82.422			-
ATOM	2334	CZ2		564		1.88		25.	546	82.929			4
ATOM	2335		TRP	564	7	70.92		27.		83.461			.
ATOM	2336	CH2	TRP	564		70.80		26.		83.279		.18	1 1
ATOM	2337	С	TRP	564		4.88			597	62.525		.66	5. E
ATOM	233B	C	TRP	564		75.90			259	82.740		.32	-
MOTA	2339	N	LYS	565		73.69			997	82.927 83.612		.00	E
ATOM	2340	CA	LYS	565		73.54			256 332	82.625		.00	÷
MOTA	2341	CB	LYS	565		73.09			886	81.791		. : 5	:
ATOM	2342	CG	LYS	565		74.24 73.82			197	E0.371		.81	ŧ.
ATOM	2343	CD	LYS	565		74.81			116	79.711		1.15	1
ATOM	2344	CE	LYS	565 565		74.85			374	80.497		5.31	-
ATOM	2345	NZ	LYS LYS	565		72.60			171	84.878		3.24	<i>₹</i>
ATOM	2346	C	LYS	565		71.8			270	85.043	1.00	2.93	3 -
ATOM	2347	0 N	LEU	566		72.8			.113	85.783	1.00	3.46	
ATOM	2348 2349	CA	LEU	566		72.1			.100	87.042	1.00	5.16	÷
ATOM	2350	CB	LEU	566		73.1	87	33.	.857	88.143	1.00	7.13	÷ .
MOTA MOTA	2351	CG	LEU	566		72.9	02	33	.890	89.641	1.00 1		5
ATOM	2352		LEU	566		74.1	21	33	. 292	90.343	1.00 1		÷
ATOM	2353		LEU	566		72.6	60		.299	90.155	1.00 1		÷
ATOM	2354	С	LEU	566		71.5			.418	87.265		6.69	•
ATOM	2355	С	LEU	566		72.1			.430	87.315		6.50	ē t
ATOM	2356	N	CYS	567		70.1			.446	87.406		7.27	-
ATOM	2357	CA	CYS	567		69.6			.738	67.658			τ. ξ
ATOM	2358	С	CYS	567		69.2			.013	69.124			:
ATOM	2359		CYS	567		69.2			.113	89.983 86.70			÷
ATOM	2360		CÄE	567		68.5 67.1			.797	66.808			1.5
MOTA	2361		CYS	567		69.0			.293	89.40			-
ATOM	2362		ARG ARG	568 568		68.6			3.777				6
ATOM	2363		ARG	568		68.			.310			17.37	÷
MOTA	2364	_	ARG	568		70.0			.829			20.45	÷
MOTA	2365 2366	_	ARG	568		71.:			711			20.67	÷
ATOM	2367		ARG	568		72.0			. 996		4 1.00	22.26	7
ATOM	2368		ARG	568		72.	587	42	2.642	91.67	1 1.0σ	22.85	÷
MOTA MOTA	2369		1 ARG	568		72.		4:	2.151	92.91			7
ATOM	237		2 ARG	568		73.		4.	3.816	91.46			7
ATOM	237		ARG	568		67.	185	3	8.399	91.08			÷
MOTA	237		ARG	568		66.			8.690			15.75	€ 8 7
ATOM	237		LEU	569			046		7.752			11.39	
ATOM	237	4 CA	LEU	569			782		7.304			6.92 2.00	÷
MOTA	237			569			005		6.101			3.41	•
MOTA	237			569			069 374		4.91			3.80	÷
MOTA	237		1 LEU	569 569			852		3.67			2.00	÷
ATOM	237		2 LEU	569			318		8.46			7.64	•
ATOM	237		LEU	569			121		9.22			6.24	?
ATOM	238		HIS	570			015		8.64			9.65	-
ATOM				570			454		9.71		1.00	10.84	€.
ATOM ATOM				570			841		10.81		55 1.00	11.04	:
ATOM				570		63.	. B20		11.54			10.31	÷
ATOM			D2 HIS	570		64	.739	2	12.49			13.10	÷
ATOM			D1 HIS	570	I	63	. 845		41.42			14.30	-
ATOM			E1 HIS	570)		.728		42.26			14.17	÷
ATOM		8 N	E2 HIS	570	}		. 285		42.92			12.65	
ATOM	231						.35		39.07			9.92	:
MOTA	1 23	90 . 0	HIS				.09		37.38			14.44 9.24	=
ATOM							. 72		39.86				:
ATON			A GLN				. 65		39.36 38.80			11.43	
10TA			B GLN				.18		38.0			13.07	
1OTA			G GLN				.15			12 100.6		21.53	
ATO			D GL				.16			37 101.3		23.69	
ATO			E1 GLN				1.11			62 101.1		22.76	
ATO			E2 GL: GLI				7.71		40.5				: :
ATO! ATO!			SLI				0.09		41.6				
ATO			i Ali				. 44		40.1		119 1.00	4.26	
ATO			CA AL				7.34		41.0				
ATO			CH AL				6.92		41.7				
ATO			AL.			5	6.21	17	40.2				
ATO			· AL				6.26		38.9				
ATO		105	N PR				5.21		40.3				
ATO	M 24		CD PP.				5.08		42.1				
ATO			CA PR				4.20		39.8		323 1.0		
ATC			CB PP				3.79			137 100. 199 100.			
ATC			CG PR				4.71		39.		377 1.0		
ATC	າຕ 2	410	C PP	3	7.3	3	3.0	- ·	٠ - د				-

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ATOM	2411	0	PRO	573	52.768	40.608	97.552	1.00 7.72
ATOM	2412	N	THR	574	52.428	38.574	98.476	1.00 8.95
ATOM	2413	CA	THR	574	51.255	38.232	97.727	1.00 10.96
ATOM	2414	CB	THP.	574	51.075	36.738	97.733	1.00 10.37 6
ATOM	2415	0G1	THE	574	52.135	36.153	96.980	1.00 14.24
ATOM	2416	CG2	THR	574	49.712	36.324	97.155	1.00 13.72 6
ATOM	2417	С	THR	574	50.119	38.852	98.515	1.00 12.85
ATOM	2418	0	THR	574	50.163	38.874	99.753	1.00 14.59 3
ATOM	2419	N	ALA	575	49.087	39.324	97.812	1.00 14.88 7
ATOM	2420	CA	ALA	575	47.934	39.946	98.467	1.00 14.50 6
MOTA	2421	CB	ALA	575	46.933	40.433	97.439	1.00 14.72 6
ATOM	2422	С	ALA	575	47.282	38.960	99.443	1.00 14.38 6
MOTA	2423	0	ALA	575	46.480	39.355	100.286	1.00 15.91 3
MOTA	2424	N	ARG	576	47.663	37.695	99.344	1.00 12.79 7
MOTA	2425	CA	ARG	576	47.178		100.189	1.00 11.82 6
ATOM	2426	CB	ARG	576	46.877	35.414	99.328	1.00 15.95 6
ATOM	2427	CG	ARG	576	45.534	35.451	98.604	1.00 20.92 6
ATOM	2428	CD	ARG	576	45.633	34.631	97.302	1.00 24.61 6
ATOM	2429	NE	ARG	576	44.350	34.081	96.848	1.00 27.37 7
ATOM	2430	CZ	ARG	576	44.171	33.438	95.687	1.00 28.99 6
ATOM	2431	NH1		576	45.188	33.261	94.833	1.00 29.46 7
ATOM	2432		ARG	576	42.979	32.928	95.391	1.00 27.90 7
ATOM	2433	C	ARG	576	48.090		101.351	1.00 9.90 5
ATOM	2434	0	ARG	576	47.843	35.177	101.972	1.00 8.14 E
ATOM	2435	N	GLY	577	49.167	36.963	101.606	1.00 10.36 7
ATOM	2436	CA	GLY	577	50.066	36.615	102.705	1.00 9.58 6
ATOM	2437	Ċ	GLY	577	51.201	35.638	102.435	1.00 11.02 6
ATOM	2438	0	GLY	577	51.959		103.356	1.00 10.42 3
ATOM	2439	N	ALA	578	51.263		101.193	1.00 11.51 7
ATOM	2440	CA	ALA	578	52.332	34.245	100.730	1.00 10.32 6
ATOM	2441	CB	ALA	578	51.842	33.360	99.617	1.00 6.95 5
ATOM	2442	C	ALA	578	53.443		100.212	1.00 10.21 6
ATOM	2443	Ö	ALA	578	53.278		100.138	1.00 9.88 8
ATOM	2444	N	VAL	579	54.597	34.593	99.905	1.00 9.95 7
ATOM	2445	CA C9	VAL	579	55.673	35.431	99.406	1.00 10.55 6
ATOM	2446		VAL	579	56.957		100.247	1.00 9.32 6
ATOM	2447		VAL	579 579	56.734		101.618	1.00 8.45 6
ATOM	2448		VAL		57.363		100.350	1.00 11.44 6
ATOM	2449	C	VAL	579	55.923	35.128	97.939	1.00 9.09 6
ATOM	2450	0	VAL	579	55.599	34.044	97.452	1.00 8.40 3
ATOM	2451	N CA	ARG ARG	580	56.460	36.104	97.229	1.00 7.06 7
ATOM ATOM	2452	CB		590	56.721	35.917	95.816	1.00 7.86 6
ATOM	2453 2454	CG	ARG ARG	580 580	55.769 55.926	36.792 36.721	94.991	1.00 8.84 6
ATOM	2455	CD	ARG	580	55.080	37.813	93.503 92.844	1.00 7.88 6
ATOM	2456	NE	ARG	580	53.652	37.517	92.913	1.00 B.7B 5
ATOM	2457	CZ	ARG	580	52.719	38.362	93.341	1.00 6.85 T
ATOM	2458		ARG	580	53.050	39.581	93.731	
ATOM	2459		ARG	580	51.470	37.952	93.466	1.00 5.12 7
ATOM	2460	C	ARG	580	58.159	36.282	95.523	1.00 7.72 &
ATOM	2461	Š	ARG	580	58.664	37.321	95.954	1.00 7.72
ATOM	2462	N	PHE	581	58.827	35.387	94.827	1.00 6.07 7
ATOM	2463	CA	PHE	581	60.200	35.596	94.458	1.00 5.52 5
ATOM	2464	CB	PHE	581	60.982	34.355	94.803	1.00 4.84 6
ATOM	2465	CG	PHE	581	61.274	34.214	96.250	1.00 4.90 5
ATOM	2466		PHE	531	60.510	33.372	97.045	1.00 3.60 8
MOTA	2467		PHE	531	62.371	34.883	96.822	1.00 5.69
ATOM	2468		PHE	531	60.835	33.191	98.390	1.00 4.44
ATOM	2469		PHE	581	62.694	34.700	98.165	1.00 5.88 8
MOTA	2470	CZ	PHE	581	61.926	33.854	98.944	1.00 5.88 6 1.00 3.43 6 1.00 5.46 6 1.00 6.33 8 1.00 6.16 7
MOTA	2471	С	PHE	531	60.287	35.939	92.961	1.00 5.46
ATOM	2472)	PHE	581	59.68€	35.101	92.194	1.00 6.33
MOTA	2473	N	TRP	522	61.037	26.844	92.525	00 6.16
ATOM	2474	CA	TRP	532	61.129	37.054	91.090	1.00 7.26
ATOM	2475	CB	TRP	582	59.861	37.778	90.589	1.00 9.34
ATOM	2476	CG	TF.P	532	59.462	38.933	91.423	1.00 7.26 1.00 9.34 1.00 10.74 1.00 11.49 1.00 11.22
ATOM	2477		TP.P	582	59.916	40.268	91.280	1.00 11.49
ATOM	2478		TP.P	582	59.366	41.017	92.359	1.00 11.22
ATOM	2479		TP.P	532	60.744	40.906		1.00 11.65
ATOM	2480		TP.P	582	58.663	28.915		1.00 11.65 6 1.00 14.19 6 1.00 12.18 1.00 12.31
MOTA	2481		TPP	532	58.604	40.165		1.00 12.18
ATOM	2482		TPP	582	59.618	42.365		1.00 12.31
ATOM	2483		TRF	582	61.001	42.247		1.00 15.91
MOTA	2484	CHZ		532	60.43€	42.973		1.00 15.91 1.00 16.33
ATOM	2485	2	TP.P	582	62.409	37.522		00 7.94
ATOM	2486	÷	TRP	532	63.219	38.299		1.00 5.37
MOTA	2487	N	CYS	583	62.55€	37.312		00 7.90
atom	2488	CA	CXS	583	63.65ē	37.766	63.334	1.00 9.15

bref2	lc.pdl	5		Thu .	Apr 25	12:	27:47	1996	33	
•			CYS !	583	63.1	54 3	B.449	•	1.00 8.52	÷
ATOM ATOM				583	62.1	43 3			1.00 8.13	.3
ATOM	2491		CYS	583	64.5		6.591		1.00 11.02	6 1 6
ATOM	2492			583	65.6		6.996		1.00 12.88	7
ATOM	2493			584	63.B		9.453 10.150		1.00 11.13	÷
MOTA	2494			584	63.5 63.2		11.612		1.00 14.00	5
MOTA	2495			584 584	62.2		2.141		1.00 22.72	3
ATOM	2496		SER	584	64.8		10.052	£4.531	1.00 11.03	5
ATOM	2497 2498		SER	584	65.8		10.485	£4.990	1.00 14.12	3
ATOM ATOM	2499		LEU	585	64.	143 3	39.357	€3.390	1.00 8.82	7
MOTA	2500		LEU	585	65.8		39.214	£2.500	1.00 7.31	÷
MOTA	2501	CB	LEU	585	65.		38.192	£1.374	1.00 5.24 1.00 2.00	6
ATOM	2502		LEU	585	65.7		36.731 35.888	21.541 20.486	1.00 2.00 1.00 2.00	6
MOTA	2503	CD1		585 585	65. 65.		36.271	€2.912	1.00 5.67	5
ATOM	2504	CD2	LEU	585	66.		40.562	81.832	1.00 8.79	5
ATOM	2505 2506	0 0	LEU	585	65.		41.282	21.508	1.00 7.56	
ATOM ATOM	2507	N	PRO	586	67.		40.929	E1.637	1.00 10.50	
ATOM	2508	CD	PRO	586			40.279	82.160	1.00 12.29	_
ATOM	2509	CA	PRO	586			42.202	80.993	1.00 11.85	
MOTA	2510	CB	PRO	586			42.304	81.191 82.416	1.00 13.83	_
ATOM	2511	CG	PRO	596		505	41.470	79.520	1.00 14.14	
MOTA	2512	C	PRO	586 586		416 B34	41.019	73.912	1.00 14.17	
MOTA	2513	0 N	PRO THR	587		691	42.985	73.957	1.00 13.17	7
ATOM	2514 2515	CA	THE	587		261	42.949	77.569	1.00 12.49	
ATOM ATOM	2516	CB	THF.	587		168	44.355	76. 9 69	1.00 15.17	
ATOM	2517		THR	587	65.	927	45.330	73.002	1.00 18.67	
ATOM	2518	CG2	THP	587		.049	44.408	75.929	1.00 17.05	
MOTA	2519	C	THR	587		.182	42.186	75.657	1.00 12.00	
MOTA	2520	O	THF.	587		.739	41.308	75.948 76.700	1.00 11.5	
MOTA	2521	N	ALA	588		.472 .513	42.530	75.849	1.00 7.8	_
MOTA	2522	CA	ALA	588 588		.896	42.342	76.320	1.00 8.9	
ATOM	2523	CB	ALA ALA	588		.435	40.425	75.700	1.00 7.3	6 5
ATOM	2524 2525	С 0	ALA	588		.825	39.894	74.681	1.00 8.3	
MOTA MOTA	2526		ASP	589		.877	39.747		1.00 7.8	
MOTA	2527		ASP	589	68	.745	38.300		1.00 7.8	
ATOM	2528		ASP	589		.173	37.684	77.976	1.00 5.2	
ATOM	2529		ASP	589		.673	37.683		1.00 5.2	
MOTA	2530		ASP	589		.088	38.045 37.299		1.00 2.0	
ATOM	2531		ASF ASF	589 589		.341	37.845		1.00 7.9	
ATOM	2532 2533		ASP	589		.080	36.659		1.00 7.8	36 5
MOTA MOTA	2534		THF.	590		. 435	38.780		1.00 8.8	
ATOM	2535		THF.	590	65	.040	38.451			
ATOM	2536		THP	590	64	.118	39.57			
ATOM			1 THE.	590		1.49€	40.80			
ATOM		B CG		590		1.269	39.721			
ATOM			THR	590		1.696	38.10 38.41			
MOTA			THF.	590		3.610 5. 59 2	37.40			_
ATOM			SER SER	591 591		5.373	37.02			
ATOM ATOM				591		6.692	36.68		1.00 13.	
ATOM				591	6	7.046				79 3
MOTA			SER	591		4.405				
ATOM	1 254	6 . 0	SER			4.456				
MOTA			SEF.			3.585			_	34 î 84 î
ATOM						2.607 1.395				26 5
ATON						0.795				45 3
40TA			SER			3.216				35 6
ATON ATON			SEF.			4.386				72 3
ATO						2.388	32.98	io €9.53		79 7
ATO						2.715				. 33
ATO	M 255	55 C		593	3 (2.86				.57 5
ATO	M 255					51.744				.76 5
ATO			D1 PHE			52.04				.27 5 .21 5
ATO			D2 PHE			60.399 61.029				.60
ATO	_		E1 PHE E2 PHE			59.38				.01
ATO			C PHE			59.68				.44
OTA ATO						63.84				. 34
ATO						64.30		77 63.15	1.00 11	
ATO					4	64.22	3 30.9			. 32
ATC	M 25	65 3	A VA			65.28				. 29
ATC	M 25	66 3	AV A	I 59	14	66.58	8 30.9	09 71.1	55OC 9	.17

bref2	1c.pd	Ъ		Thu	Apr	25	12	:27:47	1996		34	
ATOM	2567	CG1	VAL	594	6	7.08	6	31.490	69.894	1.00	11.27	ŧ
ATOM	2568	CG2	VAL	594	6	6.35	ō :	32.005	72.175	1.00	3.98	÷
MOTA	2569	С	VAL	594		4.87		29.552	72.261	1.00	6.86	€.
MOTA	2570	၁	VAL	594		4.20		30.239	73.037	1.00	9.44	7
MOTA	2571	N	PRO	595		5.28		28.308	72.572	1.00	4.06	-
ATOM	2572	CD	PRO	595 595		5.91		27.414	71.592	1.00	4.50	
ATOM ATOM	2573 2574	CA CB	PRO PRO	595·		5.04 5.62		27.55B 26.1 8 5	73.802 73.468	1.00	4.33	÷.
ATOM	2575	CG	PRO	595		5.44		26.084	72.064	1.00	4.07 2.00	₹ ₹
ATOM	2576	c	PRO	595		5.72		28.142	75.048	1.30	3.58	÷
ATOM	2577	0	PRŌ	595	6	6.95		28.077	75.180	1.00	3.03	=
MOTA	257B	N	LEU	596	6	4.92	3	28.692	75.955	1.00	3.21	-
ATOM	2579	CA	LEU	596		5.42		29.282	77.199	1.00	4.16	£
ATOM	2580	CB	LEU	596		4.67		30.596	77.561	1.00	3.39	÷
ATOM	2581	CS	LEU	596		5.38		31.870	78.068	1.00	2.00	
ATOM ATOM	2582 2583		LEU	596 596		4.50 6.64		32.639 31.534	79.002 78.783	1.00	3.47	÷
ATOM	2584	C	LEU	596		5.25		28.293	78.347	1.00	2.16 4.67	÷
ATOM	2585	ō	LEU	596		4.12		27.938	73.721	1.00	2.52	÷
ATOM	2586	N	GLU	597		6.38		27.861	78.900	1.00	4.53	-
MOTA	2587	CA	GLU	597	6	6.40	6 .	26.943	80.031	1.00	3.76	÷
ATOM	2588	CB	GLU	597		7.56		25.980	79.909	1.00	2.00	ŧ
MOTA	2589	CG	GLU	597		7.69		25.125	81.113	1.00	2.00	ŧ
ATOM	2590	CD	GLU	597		8.54		23.955	20.855	1.00	5.62	€.
ATOM ATOM	2591 2592	OE1	GLU	597 597		9.20 8.56		23.971	79.805		10.01	=
ATOM	2593	C	SLU	597		6.48		23.014 27.704	81.675 81.367	1.00	6.65	÷
ATOM	2594	ŏ	GLU	597		7.32		28.596	81.536	1.00	2.57 3.19	•
ATOM	2595	N	LEU	598		5.59		27.35B	82.296	1.00	3.03	-
ATOM	2596	CA	LEU	598		5.51		28.001	83.600	1.00	2.16	÷
ATOM	2597	CB	LEU	598	6	4.15	9	28.670	83.777	1.00	2.00	÷
ATOM	2598	CG	LEU	598	6	3.75	6	29.657	82.681	1.00	2.00	÷
ATOM	2599	CD1	LEU	598		2.27		29.702	82.601	1.00	2.00	÷
ATOM	2600			598		4.36		31.027	82.888	1.00	2.00	÷
ATOM	2601	C	LEU	598		5.76		26.988	64.700	1.00	2.92	5
ATOM	2602	0	LEU	598		5.33		25.833	84.605	1.00	2.64	=
ATOM	2603	N	ARG	599		6.46		27.428	85.736	1.00	2.34	
ATOM ATOM	2604 2605	CA CB	ARG ARG	599 5 9 9		6.80 8.25		26.580 26.115	86.862 86.710	1.00	3.62	÷
ATOM	2606	CG	ARG	599		8.47		24.611	86.512	1.00	6.78 10.90	€ €
ATOM	2607	CD	ARG	599		9.38		24.359	85.308		14.84	÷
ATOM	2608	NE	ARG	599		9.65		22.945	85.047		17.19	-
ATOM	2609	CZ	ARG	599	7	0.17	6	22.100	85.942		17.80	ŧ
ATOM	2610	NHl	AP.G	599	7	0.47	2	22.515	87.182	1.00	17.23	-
ATOM	2611	NH2		599		0.45		20.845	85.580		15.70	-
ATOM	2612	Č	ARG	599		6.71		27.367	88.150	1.00	3.41	:
ATOM ATOM	2613 2614	O N	ARG VAL	599 600		7.39 5.84		28.364 26.379	68.259 89.081	1.00	4.23	=
ATOM	2615	CA	7AL	500		5.75		27.644	90.387	1.00	2.37 2.37	:
ATOM	2616	CB	7AL	600		4.32		28.001	90.825	1.00	2.02	
ATOM	2617	CG1		600		4.33		28.512	92.248	1.30	2.00	-
ATOM	2618		VAL	600		3.73		29.035	89.917	1.00	2.00	
MOTA	2619	С	YAL	600	•	66.27	73	26.622	91.371	1.00	3.23	÷
ATOM	2620	0	VAL	600		55.74		25.525	91.426	1.00	4.11	:
ATOM	2621	N	THE	601		57.30		26.963	92.124	1.00	5.21	
ATOM	2622	CA	THE	601		57.88		26.043	93.098	1.00	6.74	***************************************
MOTA	2623	CB	THP.	601		59.29		25.601	92.688	1.00	8.50	
ATOM ATOM	2624 2625		THP.	601 601		59.22 59.89		24.939	91.430 93.684	1.00		:
ATOM	2626	C	THE	601		57.99		26.634	94.481	1.00	8.70 8.74	:
ATOM	2627	ō	THR	601		58.26		27.822	94.637		11.77	:
ATOM	2628	N	ALA	602		67. 7 6		25.792	95.484	1.00	9.57	-
MOTA	2629	CA	ALA	602	•	67.91	15	26.196	96.877	1.50	3.62	:
MOTA	2630	CB	ALA	602		67.25		25.191	97.745	1.00	3.55	•
MOTA	2631	C	ALA	602		69.40		26.180	97.153	1.00	10.39	:
MOTA	2632	C-	ALA	602		70.10		25.324	96.613	1.55	11.56	:
MOTA MOTA	2633	N.	ALA	603 603		69.87 71.29		27.069	93.036	1.30	9.78	-
ATOM	2634 2635	CA CB	ALA ALA	603		71.23 71.53		27.162 28.370	98.415 99.300	1.00	7.23 6.77	:
ATOM	2636	2	ALA	603		71.B		25.882	99.070	1.20	5.03	:
ATOM	2637	Š	ALA	603		73.0		25.785	9.320	1.11	4.90	:
ATOM	2638	N	SER	604		71.02		24.892	99.324	1.00	5.87	-
ATOM	2639	CA	SEF.	604		71.4		23.639	99.897	1.33	7.44	
ATOM	2640	CP	SER	604		70.4			100.749	1.50	5.37	:
ATOM	2641	္ငင	SER	604		69.7		22.024	99.997	1.::	5.42	;
ATOM ATOM	2642	C	SER	604		71.9:		22.689	98.777	1.00	9.18	•
ATOM ATOM	2643 2644	0	SER	604 605		72.4 71.6		21.617	99.042	1.00	11.68	:
7.2017	2074	.4		303		0	J4	23.070	97.535	2.00	1.29	

bref21	.c.pd	b		Thu	Apr	25	12	: 2	7:47	1996		35	
ATOM	2645	CA	GLY	605		71.9			262	96.378			₹ ₹
ATOM	2646	С	GLY	605		70.7			620	95.785	_		•
MOTA	2647	0	GLY	605		70.7			198	94.631 96.573	-	7.11	-
MOTA	2648	N	ALA	606		69.6			606 001	96.194		6.20	÷
MOTA	2649	CA	ALA	606		68.3 67.4			. 885	97.387		2.64	÷.
ATOM	2650	CB	ALA	606 606		67.6			.770	95.113		6.88	÷
ATOM	2651	0	ALA ALA	60 6.		67.4			974	95.234		7.80	÷
ATOM ATOM	2652 2653	N	PRO	607		67.2			.063	94.074	1.00	6.21	-
MOTA	2654	CD	PRO	607		67.4	57		.6 36	93.821	1.00	6.78	•
ATOM	2655	CA	PRO	607		66.5			.660	92.950	1.00	7.75 7.27	4 4
ATOM	2656	CB	PRO	607		66.6			.587	91.845 92.355	1.00	5.40	ŧ
MOTA	2657	CG	PRO	607		67.6			.620 .969	93.220	1.00	6.86	
MOTA	2658	0	PRO PRO	607 607		64.2			.084	93.599	1.00	6.25	1
MOTA MOTA	2659 2660	N	ARG	608		64.6			.215	92.953	1.00	6.55	
ATOM	2661	CA	ARG	608		63.2	284	23	.658	93.095	1.00	6.82	•
ATOM	2662	CB	ARG	608		63.			.105	93.591	1.00	7.55	₹ •
ATOM	2663	CG	ARG	608		63.			.320	95.066	1.00 1	11.99	
MOTA	2664	CD	ARG	608		62.			.474	95.992 95.820	1.00		-
MOTA	2665	NE	ARG	608		61.			.719 .828	96.200	1.00		ŧ
MOTA	2666	CZ	ARG	608 608		60. 61.			5.817	96.773	1.00		-
ATOM	2667		ARG ARG	608		59.			936	96.048	1.00		-
ATOM ATOM	2668 2669	C	ARG	608		62.			3.548	91.739	1.00	6.91	
MOTA	2670	0	ARG	608		61.		22	2.836	91.612	1.00	9.99	1
ATOM	2671	N	TYP	609			095		4.194	90.700	1.00	7.03	4
ATOM	2672	CA	TYP.	609			405		4.140	89.406	1.00	7.82 9.92	1
MOTA	2673	CB	TYP	609			533		5.394 5.684	89.203 90.298	1.00	11.75	÷
ATOM	2674	CC	TYR	609			54 3		6.798	91.137		12.36	•
ATOM	2675		1 TYR 1 TYR	609 609			768		7.078	92.156		13.98	₹.
ATOM ATOM	2676 2677		2 TYP	609			434		4.852	90.499	1.00	13.86	÷
MOTA	2678		2 TYP.	609		58.	494	2	5.120	91.506		13.63	•
ATOM	2679		TYP.	609			664		6.235	92.326		15.21	f E
MOTA	2680	OH		609			. 689		6.529			17.36 7.45	÷
ATOM	2681		TYP.	609			.316		4.032	88.193 88.207		10.10	•
MOTA	2682		TYR	609			.448 .803		3.416			4.17	-
ATOM	2683		HIS HIS	610 610			.536		3.308			3.51	÷
MOTA MOTA	2684 2685						.306		1.995			2.85	:
ATOM	2686						.112		1.883			2.00	
ATOM	268		2 HIS				. 692		22.830			2.00	-
ATOM	26B8		ol HIS				.346		20.681			2.00 2.00	
MOTA	2689		1 HIS				.030		20. 89 3 22.189			2.00	:
ATOM	2690		2 HIS				.250		23.45				-
ATOM	269 269		HIS				.459		22.82				÷
MOTA MOTA	269						.790		24.30	6 E3.80			•
ATOM	269						.85		24.56				:
MOTA	269		B ARC				. 941		25.70				÷
ATOM	269						. 47		25.57				
MOTA	269						3.70 7.50		26.89 26.83				-
MOTA MOTA							5.64		27.83			4.31	1
MOTA			H1 AR				6.85		28.97				-
ATOM			H2 AR		1		5.60		27.71				
ATOM		2 . C	AR				2.65		24.99				£
ATOM							3.80		25.35				-
ATOM							2.07 2.66		24.33				:
ATOM			A VA B VA				2.05 3.05		24.06				:
MOTA MOTA			B VA G1 VA				3.80		24.56				
ATOM			G2 VA				3.91		23.08				2
ATOP			AV :			ž	1.49	3 C	25.9				
ATON			. УA	L 61	. 2		0.38		25.43				
ATO			9 II				1.6		27.10			0 2.39 0 2.00	
ATON			CA II		13		9.8		27.3				
ATO			CB II CG2 II		13 13		9.2		28.2				
OTA IOTA			CG1 II		13		0.8		30.0				
ATO			CD1 II		13		0.2		31.2	41 79.1	82 1.0	0 2.00	
ATO				LE 6	13		0.9		28.5				
OTA	M 27	18			13		52.1		28.5				
ATO					14		50.0 60.2		29.1				
OTA OTA					14 14		59.6		29.4				
ATO					14		ć(ι. 4		28.1				

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ATOM	2723	CD2	HIS	614	6	1.353	28.536	71.281	1.00	2.96	÷
ATOM	2724		HIS	614		0.442		72.609	1.00	4.63	7
ATOM	2725		HIS	614		1.310		71.865	1.00	2.00	
ATOM	2726		HIS	614		1.875		71.051	1.00	6.31	5
ATOM	2727	С	HIS	614		9.580		74.664	1.00	3.58	5
ATOM	2728	ō	HIS	614		8.419		75.046	1.00	2.50	9
ATOM	2729	N	ILE	615		0.315		74.674	1.00	2.76	7
ATOM	2730	CA	ILE	615		9.717		75.108	1.00	2.55	
ATOM	2731	CB	ILE	615		0.770		75.221			5
ATOM	2732		ILE	615		0.102		75.507	1.00	2.49	÷
ATOM	2733	CG1	ILE	615		1.785		76.307	1.00	2.99	÷
ATOM	2734	CD1	ILE	615		3.067		76.351		2.00	6
ATOM	2735	c	ILE	615		8.569		74.205	1.00	2.00	ć
ATOM	2736	Ö	ILE	615		7.609		74.651	1.00	3.27	÷
ATOM	2737	N	ASN	616		8.639		72.943	1.00	5.04	3
ATOM	2738	CA	ASN	616		7.618		71.945	1.00	5.73	7
ATOM	2739	CB	ASN	616		8.205		70.513	1.00	4.76	÷
ATOM	2740	cG	ASN	616		8.860		70.236	1.00	2.00	6
ATOM	2741		ASN	616		8.410		69.399	1.00	2.00	6
ATOM	2742		ASN	616		9.954		70.910	1.00	2.00	3 7
ATOM	2743	С	ASN	616		6.287		72.124	1.00	4.60	6
ATOM	2744	0	ASN	616		5.265		71.581	1.00	6.70	3
ATOM	2745	N	GLU	617		6.280		72.989	1.00	4.63	7
ATOM	2746	CA	GLU	617		5.088		73.242	1.00		ŕ
ATOM	2747	СВ	GLU	617		5.424		73.185	1.00	5.16	
ATOM	2748	CG	GLU	617		6.381		72.086	1.00	4.92	é
ATOM	2749	CD	GLU	617		6.433		71.704		8.53	é
ATOM	2750		GLU	617		6.653		70.498		11.83	÷
ATOM	2751		GLU	617		6.276		72.575		15.40 14.68	ē
ATOM	2752	c	GLU	617		4.438		74.587	1.00		à
ATOM	2753	Š	GLU	617		3.440		74.930	1.00	4.18	5
ATOM	2754	N	VAL	618		4.995		75.354		7.74	á
ATOM	2755	CA	VAL	618		4.433		76.655	1.00	3.63	7
ATOM	2756	CB	VAL	618		5.365		77.870		2.00	5
ATOM	2757		VAL	618		5.666		77.838	1.00	2.00	6
ATOM	2758		VAL	618		6.651		77.890	1.00	2.00	6
ATOM	2759	c	VAL	618		4.119		76.727	1.00	2.00	5
ATOM	2760	ō	VAL	618		4.600		77.616	1.00	2.00	6
ATOM	2761	N	VAL	619		3.333		75.778	1.00	2.77	3 7
ATOM	2762	CA	VAL	619		2.970		75.792	1.00	2.00 3.10	6
ATOM	2763	СВ	VAL	619		2.765		74.407	1.00	2.32	6
ATOM	2764	CG1	VAL	619		2.741		74.449	1.00	2.43	5
ATOM	2765	CG2		619		3.884		73.519	1.00	7.61	6
ATOM	2766	ε	VAL	619		1.700		76.589	1.00	4.11	5
ATOM	2767	0	VAL	619		0.817		76.610	1.00	6.41	3
ATOM	2768	N	LEU	620		1.639		77.268	1.00	2.53	7
ATOM	2769	CA	LEU	620		0.492		78.080	1.00	3.37	é
ATOM	2770	CB	LEU	620		0.702		79.554	1.00	3.39	÷
ATOM	2771	CG	LEU	620		9.613		80.438	1.00	3.95	6
ATOM	2772	CD1		520		0.233		81.775	1.00	5.62	á
ATOM	2773		LEU	620		8.306		80.529	1.00	3.31	é
ATOM	2774	С	LEU	620		0.382		77.920	1.00	5.44	- 6
ATOM	2775	Ş	LEU	620		0.858		78.736	1.00	7.07	ā
MOTA	2776	N	LEU	621		9.739		76.834	1.00	7.07	7
MOTA	2777	CA	LEU	621	4	9.549		76.465	1.00	5.70	5
MOTA	2778	CB	LEU	621	4	8.832	41.498	75.111	1.00	5.58	6
ATOM	2779	CG	LEU	621		9.469		73.845	1.00	2.00	5
MOTA	2780	. CD1		621	4	18.395	40.832	72.831	1.00	2.42	5
ATOM	2781	CD2	LEU	621	5	0.545	41.903	73.377	1.00	2.00	6
MOTA	2782	С	LEU	621	4	8.730	42.253	77.427	1.00	7.59	ó
ATOM	2783	5	LEU	621	4	7.941	41.728	78.198	1.00	8.04	3
ATOM	2784	N .	ASP	522	4	8.926	43.565	77.355	1.00	11.43	3 7
ATOM	2785	CA	ASF	622	4	8.148	44.513	78.128		10.55	÷
ATOM	2786	CB	ASP	622	4	18.678	45.938	77.968	1.00	9.98	á
ATOM	2787	20	ASP	522		19.746	46.300	73.963		11.16	5
ATOM	2788		ASF	622		0.398	47.342	78.724		12.42	5
ATOM	2789		ASF	622		19.927	45.580	79.976		11.12	ą
ATOM	2790	0	ASF	622	4	6.855	44.429	77.336		10.98	5
ATOM	2791	2	ASP	622		6.867		75.152		11.16	3
ATOM	2792	33	ALA	623	4	15.754	44.808	77.965		13.11	,
ATOM	2793	CA	ALA	623	4	44.452	44.764	77.326		12.49	÷
ATOM	2794	CB	ALA	623	4	43.375	44.723	78.402		13.24	.5
ATOM	2795	2	ALA	623		44.267		75.399		10.77	-5
ATOM	2796	5	ALA	523	4	45.013	46.953	76.489		11.45	3
ATOM	2797	N	PRO	624		43.311		75.462	1.00		7
ATOM	2798	CD	PRC			12.60		75.175	1.00		-5
ATOM	2799	CA	PP.C	624		42.969		74.486	1.00		.5
MOTA	2800	CB	PRO	624	4	41.933	3 46.241	73.632	00		ŕ

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•	2801		PRO	624	42.33			73.736 75.095	1.00 9.96 5 1.00 10.98 5
	2802		PRO	624	42.36			76.056	1.00 13.90
	2803		PRO	624	41.59		3.139 3.352	74.518	1.00 11.27
ATOM	2804		VAL	625	42.69 42.19		3.532 3.638	74.969	1.00 8.57 5
ATOM	2805	CA	VAL	625	43.2		1.676	75.160	1.00 8.17 5
MOTA	2806	CB	VAL	625 625	44.0	_	1.324	76.386	1.00 10.17 5
MOTA	2807	CG1 CG2		625	44.1	_	1.744	73.933	1.00 6.41
ATOM	2808		VAL	625	41.1		1.193	73.950	1.00 11.00
MOTA	2809	င ၁	VAL	625	40.7		0.513	72.970	1.00 11.35
MOTA	2810 2811	N	GLY	626	40.6		2.392	74.243	1.00 10.53
ATOM	2812	CA	GLY	626	39.6	83 5	3.098	73.389	1.00 12.11
ATOM	2813	c	GLY	626	38.3	96 5	2.482	72.843	1.00 14.18
MOTA	2814	3	GLY	626	37.9	06 5	2.907	71.775	1.00 14.32 3
ATOM	2815	N	LEU	627	37.8	19 5	1.522	73.565	1.00 16.36
MOTA	2816	CA	LEU	627	36.5	76 5	0.879	73.112	1.00 17.03 6
MOTA	2817	CB	LEU	627	36.1	.38 4	9.789	74.092	1.00 13.89 5
ATOM	2818	CG	LEU	627	34.9	46 4	8.955	73.631	1.00 13.26
ATOM	2819		LEU	627	35.3	399 4	8.124	72.467	1.00 15.73
MOTA	2820		LEU	627	34.4	121 4	18.034	74.740	1.00 12.93 6
	2821	2	LEU	627	35.	115	1.869	72. 92 8	1.00 18.27 6
ATOM ATOM	2822	5	LEU	627	35.	007 3	52.548	73.881	1.00 17.62 3
ATOM	2823	N	VAL	628	34.	954 5	52.005	71.682	1.00 19.54 ?
ATOM	2824	CA	VAL	628	33.		52.862	71.355	1.00 19.76
ATOM		CB	VAL	628	34.	166	54.119	70.490	1.00 18.01 5
MOTA	2825		VAL	62B	34.		55.151	71.318	1.00 19.05
MOTA	2826		VAL	628	34.		53.723	69.244	1.00 18.46
MOTA	2827		VAL	628			52.009	70.609	1.00 21.37 5
MOTA	2828	5	VAL	628			51.171	€9.740	1.00 19.35
ATOM	2829	О N	ALA	629			52.157	71.036	
MOTA	2830		ALA	629			51.453	70.440	
MOTA	2831	CA	ALA	629		532	50.850	71.531	1.00 25.97
ATOM	2832			629		593	52.496		
ATOM	2833		ALA	629		684	53.693		
MOTA	2834		ALA			823	52.061		
ATOM	2835		ARG	630		014	52.979		
MOTA	2836			630			53.703		
MOTA	2837	CB		630		.873	55.154		
ATOM	2838	3 CG		630		.087			
ATOM	2839) CD		630		.565	56.016		
ATOM	2840			630		.366	57.461		•
ATOM	2841			630		. 627	58.112 57.460		
ATOM	2842		11 ARG	630		.108	59.440		
MOTA	284		12 ARG	630		.421	52.308		
MOTA	284		ARG	630		.867	51.13		
MOTA	284		ARG			.945	53.04		
MOTA	284					.787	52.49		· · · · · · · · · · · · · · · · · · ·
MOTA	284					.650	53.26		
MOTA	284					.379	52.40		
ATOM	284					.269			·
ATOM	285		D1 LEU			2.275	50.96	_	
MOTA	285	1 2	D2 LEU		_	2.351	52.32		_
ATOM	285	2 0	LEU			1.826	52.77		
MOTA	285	3 O	LEU			1.739	53.91		
ATOM			AL		_	5.094	51.75		
MOTA			A ALI			5.170	51.97		
ATOM	_		B AL		_	5.601	50.69		
ATOM			AL	A 63.	_	3.771	52.42		
ATOM		58 ° C	AL	A 63		2.964	51.60		
ATOM			AS:	P 63		3.542	53.70		
ATON			A AS		3 2	2.239	54.3		
ATON			SA ES		3 2	2.438	55.88		
ATON			G AS		3 2	2.352	56.7		
ATO			DI AS			1.778	56.3		
ATON			D2 AS			2.852	57.9	77 63.2	
ATO			C AS		-	1.466		94 60.9	
ATO) AS		_	0.253		66 60.9	
ATO			N GI			2.137			
OTA			CA GI			1.428		65 58.5	
			CF GI			22.349			
ATO			CG GI			22.847			
ATO			CD GI			23.766			
ATO			DE1 GI			24.012			
ATO		72	DE2 G			24.29			
ATC		373				20.91			
ATC		374				20.91			
ATC		375				21.46			
ATC		376							
ATC		877			35 35	21.06			
TA	DM 21	B78	CB S	ER 6	35	22.28	6 48.	020 36.	J. 1.00 90.00

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ATOM	2879	OG	SER	635	23.16	9 49.037	60.063	1.00 90.00 3
ATOM	2880	c	SER	635	20.32		60.435	1.00 90.00 5
ATOM	2881	0	SER	635	19.39		60.437	
ATOM	2882	N	GLY	536	20.78	_		
ATOM	2883	CA	GLY	636	20.21		61.488	
ATOM	2884	C	GLY	636	20.21		62.821	1.00 90.00 8
ATOM	2885	o	GLY	636			63.586	1.00 90.00 5
ATOM	2886	N	HIS		20.54		63.790	1.00 90.00 &
				637	22.20		64.010	1.00 29.39 7
ATOM ATOM	2887	CA	HIS	637	22.92		64.847	1.00 28.30 8
	2888	CB	HIS	637	23.19		64.148	1.00 27.49
MOTA	2889	CC	HIS	637	23.91		62.796	1.00 26.32 €
ATOM	2890		HIS	637	25.12		62.400	1.00 26.14 5
ATOM	2891		HIS	637	23.33		61.665	1.00 26.56 7
ATOM	2892		HIS	637	24.17		60.659	1.00 26.93 6
ATOM	2893		HIS	637	25.24		61.079	1.00 26.35
ATOM	2894	C	HIS	637	24.22		65.427	1.00 27.39 6
ATOM	2895	0	HIS	637	24.50		65.452	1.00 27.46 3
MOTA	2896	N	VAL	638	24.92		65.868	1.00 25.98 7
ATOM	2897	CA	VAL	638	26.11		66.646	1.00 22.67 5
ATOM	2898	CB	VAL	638	26.16		67.730	1.00 23.93 €
MOTA	2899		VAL	638	26.96		68.963	1.00 24.68 5
ATOM	2900		VAL	638	24.78		68.251	1.00 23.20 5
ATOM	2901	C	VAL	638	27.42		65.877	1.00 21.16 6
ATOM	2902	0	VAL	638	27. 7 6		65.236	1.00 17.80 E
ATOM	2903	Ŋ	VAL	639	28.12	9 48.808	65.940	1.00 19.71 7
ATOM	2904	CA	ANT	639	29.41		65.309	1.00 21.49 5
atom	2905	CB	VAL	639	29.36	2 49.967	64.127	1.00 22.97 క
ATOM	2906	CG1	VAL	639	30.36	3 51.140	64.296	1.00 22.32 5
ATOM	2907	CG2	VAL	639	29.53	11 49.189	62.796	1.00 21.09 6
ATOM	2908	С	VAL	639	30.50	3 49.131	66.402	1.00 18.72 6
ATOM	2909	0	VAL	639	30.56	9 50.164	67.103	1.00 15.61 3
ATOM	2910	N	LEU	640	31.24		66.588	1.00 17.29 7
ATOM	2911	CA	LEU	640	32.31		67.567	1.00 15.07 6
ATOM	2912	CB	LEU	640	32.29		69.002	1.00 11.06 5
ATOM	2913	CG	LEU	640	31.94		69.398	1.00 9.33 6
MOTA	2914	CD1	LEU	640	30.75		69.940	1.00 6.96 6
ATOM	2915		LEU	640	31.70		69.328	1.00 7.60 5
ATOM	2916	С	LEU	640	33.72		67.106	1.00 15.19 6
ATOM	2917	0	LEU	640	34.31		66.393	1.00 13.52
MOTA	2918	N	ARG	641	34.32		67.616	1.00 16.40 7
ATOM	2919	CA	ARG	641	35.71		67.269	
ATOM	2920	CB	ARG	641	35.74		66.406	
ATOM	2921	CG	ARG	641	36.50	_		1.00 18.96 6
ATOM	2922	CD	ARG	641	35.74		65.100	1.00 23.80 5
ATOM	2923	NE	ARG	641	34.64		63.884	1.00 25.92 6
MOTA	2924	CZ					63.502	1.00 26.12 7
ATOM	2925		ARG	641	33.44		63.085	1.00 27.21 6
			ARG	641	33.17		63.013	1.00 24.02
ATOM	2926		ARG	641	32.53		62.685	1.00 23.76
ATOM	2927	C	ARG	641	36.63		68.527	1.00 17.87 6
MOTA	2928	0	ARG	641	36.11		69.655	1.00 19.51 3
ATOM	2929	N	TRP	642	37.9		68.366	1.00 16.84
ATOM	2930	CA	TRP	642	38.92		69.515	1.00 14.61 5
ATOM	2931	CB	TRP	642	38.7		70.453	1.00 13.71 5
ATOM	2932	CG	TRP	642	39.10		63.819	1.00 9.75 5
MOTA	2933		TRP	642	38.20		69.133	1.00 10.16 #
ATOM	2934		TPP	642	38.92		68.814	1.00 10.08 6
ATOM	2935		TPP	642	36.85		€8.760	1.00 8.27 6
ATOM	2936			642	40.30		69.860	1.00 7.42 8
MOTA	2937		TRP	642	40.20	08 45.37?	69.267	1.00 7.42 £ 1.00 10.16 7
atom	2938		TRP	642	38.34	45 44.116	68.150	1.00 8.53 -
ATOM	2939	CZ3	TRP	642	36.21	39 45.374	68.098	1.00 7.26 €
ATOM	2940	CH2	TRP	642	37.0	35 44.225	67.803	1.00 7.13 4
MOTA	2941	С	TPF	642	40.4		69.178	1.00 15.14 6
ATOM	2942	0	TRP	542	40.7		68.006	1.00 17.51
ATOM	2243	N	LEU	643	41.2		70.207	1.00 17.51 3 1.00 13.07
ATOM	2944	CA	LEU	643	42.7		70.039	1.00 13.34 5
ATOM	2945	CB	LET	643	43.3		70.676	1.00 9.27 6
ATOM	2946	CG	LEU	643	42.8		70.081	1.00 9.05
ATOM	2947		LEU	643	43.7		70.583	1.00 7.00 5
ATOM	2948		LEU	643	43.0		68.601	1.00 9.98 5
ATOM	2949	c	LEU	643	43.5		70.662	1.00 15.42 5
ATOM	2950	ō	LEU	643	43.0			
MOTA	2951	N	PRO	644	44.6		71.697	
ATOM	2952	CD	PRC	644	45.2		70.059	2000
ATOM	2953	CA	PRO	644	45.4		68.817	1.00 15.21 5
ATOM	2954	CB	PRC	644	46.4		70.556	1.00 14.66
ATOM	2955	CG	PRC	644	46.6		69.412	1.00 15.17
ATOM	2956	C	PRO	644	46.1		68.867	1.00 15.08
		-		V 71 72	70.1	92 47.793	71.851	1.00 11.57

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ATOM	2957	o	PRO	644		6.148		.978	72.209	1.00 12.33
ATOM	2958		PRO	645		16.806		.824	72.588	1.00 10.67 7 1.00 10.47 6
MOTA	2959	CD	PRO	645		16.832 17.530		.392	73.851	1.00 9.59 6
MOTA	2960	CA	PRO	645 645		18.279		.746	74.038	1.00 10.22 5
ATOM	2961	CB CG	PRO PRO	645		47.321		.742	73.502	1.00 9.51 5
ATOM ATOM	2962 2963	c	PRO	645		48.475		3.178	73.572	1.00 9.51 5
ATOM	2964	ō	PRO	645		49.21		3.142	72.605	1.00 11.71 3 1.00 9.63 7
MOTA	2965	N	PRO	646		48.43		9.229	74.375	1.00 9.63 7 1.00 9.62 6
ATOM	2966	CD	PRO	646		47.68		9.431	75.618 74.105	1.00 9.90
MOTA	2967	CA	PRO	646		49.33 49.00		0.350 1.345	75.217	1.00 9.95
ATOM	2968	CB	PRO	646 646		47.61	_	0.941	75.674	1.00 11.92 6
ATOM	2969	CG	PRO PRO	646		50.BO	-	9.956	74.116	1.00 13.01 5
ATOM	2970 2971	0	PRO	646		51.20		8.918	74.679	1.00 14.24 5
ATOM ATOM	2972	N	GLU	647		51.62		0.786	73.470	1.00 13.38 7 1.00 14.58 5
ATOM	2973	CA	GLU	647		53.04		0.546	73.383 74.552	1.00 14.58 5 1.00 15.62 5
ATOM	2974	CB	GLU	647		53.75 53.78		1.217	74.380	1.00 19.18
MOTA	2975	CG	GLU	647 647		54.23		3.470	75.640	1.00 20.10 6
MOTA	2976 2977	CD	GLU	647		53.64		3.215	76.715	1.00 22.78
ATOM	2978		GLU	647		55.17	75 5	4.305	75.563	
atom Atom	2979	č	GLU	647		53.48		19.082	73.218	
ATOM	2980	0	GLU	647		54.50		18.697	73.795	
ATOM	2981	N	THR	648		52.7		48.316	72.384	
ATOM	2982	CA	THP	64B		53.0		46.899 45. 9 84	72.062 72.452	
MOTA	2983		THR	648		51.8		46.119	73.852	
ATOM	2984		THR THR	648 548		52.1		44.533	72.141	1.00 8.04 5
MOTA	2985 2986		THR	648		53.2		46.761	70.534	1 1.00 9.27
MOTA MOTA	2987		THR	_		52.5		47.370		
ATOM	2988		PRO			54.3		45.968		
MOTA	2989		PRO			55.3		45.245		
ATOM	2990) CA				54.6		45.819		
MOTA	2991					56.1 56.2		44.592	-	
MOTA	2997					53.8		44.707		
MOTA	2993		PRO			52.9		44.10		5 1.00 9.10 8
ATOM	2994 2995		MET			54.2		44.40	66.83	
MOTA MOTA	299	_				53.6	645	43.36		
ATOM	299				0	54.		41.96		
ATOM	299					55.		41.83		
ATOM	299					56.		40.14		
MOTA	300		E ME'			52.		43.35		
ATOM	300 300		ME'			51.		42.28		
MOTA MOTA						51.	581	44.54		
MOTA		-			1		136	44.80		
ATOM			в тн				858	46.19		
ATOM			G1 TH				419	47.19		
ATOM			G2 TH				364 353	46.50		
ATOM		-					309	43.26		
MOTA MOTA					52		866	43.47	78 63.8	
ATON			A SE		52		.110	42.62		
MOTA			B SE		52		.510	42.94		
MOTA			G SI		52		.405 .235	41.99		
ATO					52 52		.034	40.2		74 1.00 9.34
ATO					53		.523	40.7		90 1.00 7.77
OTA OTA					53		.584	39.3		
ATO					53		.991	39.0		
ATO					53		.892	3B.9		
ATO		20	CD2 H	IS 5	53		. 285			
ATO			ND1 H		53		.471			
ATO			CE1 H		53		.071			
ATO			NE2 H		53 53		.476			
ATO ATO)24)25			533		.989		44 65.	994 1.00 5.90
ATO		026			554		3.046	40.2	34 66.	
ATC		027			554		7.072			
ATC		028	CB I	LE (654		7.059			
ATC	M 3	029	CG2 I		654		6.252			653 1.00 5.93 760 1.00 3.24
ATC		030	CG1 I		654 654		8.469 8.560			131 1.00 2.00
ATO		031	CD1		654 654		5.63			156 1.00 5.10
TA TA		032 033			654		4.98		508 65.	395 1.00 7.39
ATC		034			655		5.21			713 1.00 5.70

bref2	1c.pd	ь		Thu	Apr 25 1	2:27:47	1996	40	
ATOM	3035	CA	ARG	655	43.856	38.107	67.582	1.00 4.70	5
ATOM	3036	СВ	ARG	655	43.947	36.608	67.851	1.00 6.54	6
ATOM	3037	CG	ARG	655	42.732	35.835	67.393	1.00 12.78	5
ATOM	3038	CD	ARG	655	42.923	35.234	66.013	1.00 19.16	÷
MOTA	3039	NE	ARG	655	41.690	35.243	65.243	1.00 25.22	7
ATOM	3040	CZ	ARG	655	41.487	34.509	64.155	1.00 28.18	5
ATOM	3041		ARG ARG	655 655	42.441	33.699	63.683	1.00 29.93	7
atom atom	3042 3043	C	ARG	655	40.343 43.012	34.523 38.786	63.465 68.687	1.00 30.11 1.00 4.93	7 6
ATOM	3044	ŏ	ARG	655	43.561	39.225	69.706	1.00 4.93 1.00 4.78	9
ATOM	3045	N	TYR	656	41.706	38.916	68.485	1.00 3.05	7
ATOM	3046	CA	TYR	656	40.852	39.533	69.491	1.00 4.57	6
MOTA	3047	CB	TYR	656	40.315	40.886	69.041	1.00 5.74	6
ATOM	3048	CG	TYR	656	41.339	41.973	69.131	1.00 11.08	6
ATOM	3049		TYP	656	41.994	42.423	67.995	1.00 11.86	6
ATOM	3050	CE1		656	43.029	43.341	68.077	1.00 13.79	6
ATOM ATOM	3051 3052		TYR	656 656	41.736 42.779	42.482 43.407	70.366	1.00 13.83	6
ATOM	3053	CZ	TYR	656	43.422	43.407	70.461 69.307	1.00 14.75	6 6
ATOM	3054	OH	TYR	656	44.498	44.701	69.373	1.00 19.33	8
ATOM	3055	С	TYR	656	39.693	38.646	69.848	1.00 7.31	5
ATOM	3056	0	TYP	656	39.504	37.608	69.210	1.00 7.58	ā
ATOM	3057	N	GLU	657	38.967	39.048	70.905	1.00 9.63	7
ATOM	3058	ÇA	GLU	657	37.776	38.359	71.431	1.00 9.06	5
ATOM	3059	CB	GLU	657	38.109	37.385	72.555	1.00 11.39	6
ATOM ATOM	3060 3061	CD	GLU GLU	657 657	36.874	36.766	73.217	1.00 14.76	6
ATOM	3062	CE1		657	36.755 36.157	35.254 34.838	72.977 71.945	1.00 17.29 1.00 19.32	6 8
ATOM	3063		GLU	657	37.245	34.472	73.826	1.00 19.52	8
ATOM	3064	С	GLU	657	36.827	39.366	72.006	1.00 10.04	6
ATOM	3065	0	GLU	657	37.163	40.033	72.985	1.00 8.78	8
ATOM	3066	N	VAL	658	35.635	39.428	71.412	1.00 13.32	7
ATOM	3067	CA	VAL	658	34.550	40.334	71.819	1.00 15.04	6
ATOM	3068	CB	VAL	658	33.826	40.908	70.578	1.00 17.13	6
ATOM	3069		VAL	658	32.355	41.228	70.903	1.00 18.15	6
MOTA MOTA	3070 3071		VAL VAL	658	34.552	42.151	70.055	1.00 15.29	6
ATOM	3072	0	VAL	658 658	33.518 33.025	39.602 38.519	72.697 72.336	1.00 15.57 1.00 16.39	6
ATOM	3073	N	ASP	659	33.168	40.225	73.818	1.00 15.80	8
MOTA	3074	CA	ASP	659	32.217	39.660	74.762	1.00 16.22	6
MOTA	3075	CB	ASP	659	32.857	39.583	76.152	1.00 18.33	6
ATOM	3076	CG	ASP	659	31.841	39.320	77.262	1.00 17.02	6
MOTA	3077		ASP	659	31.70€	40.220	78.127	1.00 16.96	8
ATOM	3078		ASP	659	31.191	38.238	77.248	1.00 15.05	8
ATOM ATOM	3079 3080	0	ASP ASP	659 659	30. 9 59 30. 94 6	40.488 41.480	74.877 75.641	1.00 17.09	6
ATOM	3081	N	VAL	660	29.924	40.096	74.127	1.00 16.55	3
ATOM	3082	CA	VAL	660	28.623	40.775	74.150	1.00 18.10	÷
MOTA	3083	CB	VAL	660	27.835	40.550	72.857	1.00 15.37	5
ATOM	3084	CG1	VAL	660	28.760	40.397	71.683	1.00 16.34	5
ATOM	3085	CG2	VAL	660	26.931	39.368	72.990	1.00 15.04	5
ATOM	3086	С	VAL	660	27.768	40.299	75.335	1.00 20.40	5
ATOM	3087	0	VAL	660	27.719		75.635	1.00 21.69	8
ATOM	3088	N	SER	661	27.018	41.218	75.943	1.00 22.33	7
ATOM	3089	CA	SER	661	26.210	40.865	77.104	1.00 23.37	6
atom atom	3090 3091	CB OG	SER SER	661 661	27.146 28.007	40.683 39.569	78.308 78.169	1.00 23.56	6
ATOM	3092	. c	SER	661	25.132	41.882	77.544	1.00 25.08	8 6
ATOM	3093	ò	SER	661	24.814	42.901	76.839	1.00 24.57	ล
MOTA	3094	N	ALA	662	24.676		78.784	1.00 26.02	ž
MOTA	3095	CA	ALA	662	23.690		79.598	1.00 23.48	-5
ATOM	3096	CB	ALA	662	23.909		79.493	1.00 24.66	5
ATOM	3097	c	ALA	662	22.242		79.339	1.00 22.08	.5
MOTA	3098	0	ALA	662	21.935		79.266	1.00 16.69	:3
atom atom	3099 3100	N CA	GLY	663 663	21.367		79.300	1.00 23.15	7
ATOM	3100	C	GLY GLY	663	19.936 19.124		79.047 80.038	1.00 24.87	5
ATOM	3102	Ö	GLY	663	18.542		73.649	1.00 23.53	ર્ક સ
ATOM	3103	N	ASN	664	19.032		81.277	1.00 24.09	7
ATOM	3104	CA	ASN	654	18.317		82.410	1.00 25.56	•
ATOM	3105	CF	ASN	664	17.157	42.706	82.938	1.00 27.33	ń
ATOM	3106	CG	ASN	664	15.907		82.013	1.00 28.05	6
ATOM	3107		ASN	664	15.791		81.114	1.00 29.36	3
atom atom	3108		ASN	664	14.939		82.294	1.00 26.86	-7
ATOM	3109 3110	c o	ASN ASN	664 664	17.831 16.976		82.334	1.00 25.78	15
ATOM	3111	N	GLY	665	18.350		81.488 83.243	1.00 25.92	8
ATOM	3112	CA	GLY	665	17.916		82.294	1.00 24.29	.5
									•

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ATOM	3113	С	GLY	665	18.		37.239	82.23		00 23.94	ē ā
ATOM	3114			665	18.		36.011	82.45		00 24.01 00 22.31	7
MOTA	3115			666	18.		37.805 37.054	81.04		00 22.71	5
MOTA	3116			666	19. 19.		37.724	78.69		00 21.95	5
ATOM	3117		ala Ala	666 666	20.		37.166	80.57	7 1.	00 24.38	5
MOTA	3118 3119	с 0	ALA	666	21.		38.225	81.07		00 25.18	ð
MOTA MOTA	3119	N	GLY	667	21.		36.036			00 25.52	7
ATOM	3121	CA	GLY	667		941	36.058	81.15		00 26.48	5 5
MOTA	3122	С	GLY	667		838	35.946			00 28.11	3
MOTA	3123	0	GLY	667		789	35.145 36.689			00 28.73	7
MOTA	3124	N	SER	668		483 256	36.669			00 28.04	6
ATOM	3125	CA CB	SER SER	668 668		634	37.605		7 1.	00 28.80	6
MOTA MOTA	3126 3127	OG	SER	668		312	37.574	75.27		.00 24.54	8
ATOM	3128	c	SER	668		597	37.209			.00 27.60	6 8
ATOM	3129	0	SER	668		. 647	38.220			.00 27.37 .00 26.59	7
ATOM	3130	N	VAL	669		. 623	36.397 36.71			.00 23.08	6
MOTA	3131	CA	VAL	669 669		.049 .665	35.974			.00 20.59	6
ATOM	3132	CB	VAL VAL	669		.460	34.48			.00 19.42	5
MOTA MOTA	3133 3134		VAL	669		.175	36.31	6 79.4		.00 20.06	6
MOTA	3135	c	VAL	669	28	.668	36.26			.00 21.55	5
ATOM	3136	0	VAL	669		.846	35.88			.00 20.19	8 7
ATOM	3137	N	GLN	670	_	.845	36.40			.00 20.21	6
ATOM	313B	CA	GLN	670		.193	36.00 36.23			.00 17.59	6
ATOM	3139		GLN	670 67 0		.005	35.56	_	-	.00 22.13	5
ATOM	3140 3141		GLN GLN	670		.933	36.43		02 1	.00 22.70	6
MOTA MOTA	3142		GLN	670		.500	37.48			.00 24.66	8
MOTA	3143		GLN	670		.912	35.99			1.00 23.69	7 8
ATOM	3144	C	GLN	670		.519	36.58 37.78			1.00 17.46 1.00 15.56	8
MOTA	3145		GLN	670		9.792 9.332				1.00 15.69	7
ATOM	3146		ARG ARG	671 671		1.631				1.00 16.60	6
MOTA MOTA	3147 3148		ARG	671		2.67B				1.00 17.57	6
ATOM	314	_	ARG	671	3:	2.946				1.00 19.96	6
ATOM	3150		ARG	671		2.493				1.00 18.73	6 7
ATOM	315		ARG	671		2.986				1.00 19.78 1.00 19.40	
MOTA	315			671		3.863 4.370				1.00 17.08	_
MOTA	315	-	1 ARG 2 ARG	671 671		4.304				1.00 17.95	_
MOTA MOTA			ARG	671		1.869	_		158	1.00 18.54	
ATOM	_		ARG	671	3	1.425			645	1.00 20.62	
ATOM			VAL	672		2.57			460	1.00 18.16	
ATOM				672		2.87			049 160	1.00 15.90	
ATOM				672 672		2.07		_	682	1.00 17.58	
ATOM			1 VAL	672		2.72			133	1.00 17.8	
ATOM ATOM	_	- :	VAL	672	_	4.37		38 68.	849	1.00 14.2	
ATOM			VAL	672		34.96			358	1.00 14.1	
ATON			GLU	673		35.01			184	1.00 13.3	
ATON				673		36.43 36.90			.911 .150	1.00 17.9	
ATO				673 673		36.62			. 601	1.00 21.0	7 5
ATO: ATO:						36.99		299 64	.759	1.00 22.5	
ATO			E1 GLU		,	36.96			.300	1.00 20.1	
ATO			E2 GLU		-	37.27			.537	1.00 23.5	
ATO						36.64 35.68			.978 .456	1.00 15.6	
ATO						37.89			.708	1.00 15.7	3 7
ATO			ILE A ILE			38.2		-	.790	1.00 15.3	
ATO ATO			B ILE			38.34			.498	1.00 16.7	12 ∻
ATO			G2 ILE			38.7			.483	1.00 15.	0 6
ATO			G1 ILE	67		37.0			.289	1.00 15.1	
ATO			D1 ILE			35.8			.489 5.198	1.00 12.0	
ATO			ILI			39.5 40.5			5.909	1.00 15.	
ATO			O ILI			39.7			3.884	1.00 18.	
ATC ATC			N LET			41.0			3.251	1.00 16.	13 -
ATC			CB LE			40.B	46 37	.553 6	1.744	1.00 16.	02 მ
ATC		184 (CG LE	ย 67	5	40.3			1.359	1.00 17.	
ATC	OM 3:	-	CD1 LE			38.7			1.326 0.014	1.00 13.	
ATO			CD2 LE			40.9			3.585	1.00 16.	
ATC ATC			C LE O LE			41.5			3.920	1.00 16.	45
AT			N GL		76	43.2	40 38	.587 6	3.521	1.00 14.	67
TA			CA GL		76	44.3	316 39	.514 6	3.829	1.00 12.	70

bref	21c.p	đb		Thu	Apr	25	12:27:47	1996		42	
MOTA	3191	СВ	GLU	676	4	5.667	38.907	63.526	1.00	12.08	ŧ
ATOM	3192	CG	GLU	676		5.627		62.478		11.18	•
ATOM ATOM	3193 3194	CD	GLU	676		5.494		63.080		13.77	Ę.
ATOM	3195	OE2		676 6 76		6.538 4.367		63.546		16.32	:
ATOM	3196	c	GLU	676		4.268		63.108 63.146		13.00 12.13	;
ATOM	3197	0	GLU	676		3.569		62.159		12.13	•
ATOM	3198	N	GLY	677		5.030	41.772	63.699		11.52	3
ATOM	3199	CA	GLY	677		5.121		63.145		11.07	:
atom atom	3200 3201	0	GLY	677 677		3.796		62.961		11.96	=
ATOM	3202	N	ARG	678		3.770 2.700		62. 5 23		14.32	:
MOTA	3203	CA	ARG	678		1.387		63.174		12.98 14.43	÷
MOTA	3204	CB	ARG	678		0.342		62.927		13.34	•
MOTA	3205	CG	ARG	678		9.529		61.695		15.05	ŧ
MOTA MOTA	3206 3207	CD NE	ARG	678 678		0.401		60.504		17.70	€ 7
ATOM	3208	CZ	ARG	678 678		1.014 1.887		60.643		22.61	
ATOM	3209		APG	678		2.274		59.787 58.700		23.28 22.06	€
- ATOM	3210	NH2	ARG	678		2.380		60.037		25.26	-
ATOM	3211	С	ARG	678		1.001		64.420		14.43	Ę
ATOM ATOM	3212 3213	o N	ARG THR	678		1.199		65.529		15.07	3
ATOM	3214	CA	THE	679 679		0. 46 2 0.027		64.249		13.15	
ATOM	3215	CB	THP	679		0.996		65. 39 0		14.13	Ę
ATOM	3216	OG1		679		1.204		64.448		14.19 17.57	÷
ATOM	3217	CG2	THE	679		2.332		66.229		13.59	÷
ATOM	3218	С	THP	679		8.637		65.182		16.43	:
ATOM	3219	0	THE	679		8.393		65.540		15.23	=
MOTA MOTA	3220 3221	N CA	SLU	680		7.732		64.604		18.09	
MOTA	3222	CB	GLU	680 680		6.358 6.2 8 9		64.332		19.04	£.
ATOM	3223	CG	GLU	680		6.140		63.128 61.755		18.69	•
ATOM	3224	CD	GLU	680		5.086		60.847		18.32 18.05	
ATOM	3225		GLU	680	34	4.342		60.138		16.53	•
ATOM	3226		GLU	680		5.019		60.825		14.40	3
ATOM ATOM	3227 3228	0	GLU	680		5.489		64.076		21.29	5
ATOM	3229	N	CYS	680 681		5.887 4.299		63.364		22.54	3
ATOM	3230	CA	CYS	681		3.382		64.654 64.498		22.91 24.61	-
ATOM	3231	CB	CYS	681		3.617		65.603		26.42	5
ATOM	3232	SG	CYS	681	3:	2.134		66.606		26.71	<u>:</u>
ATOM	3233	C	CYS	681		1.958		64.540	1.00	24.30	•
ATOM ATOM	3234 3235	O N	CYS VAL	681 682		1.579		65.448		23.84	÷
ATOM	3236	CA	77.1	682		1.181 9.818		63.517		21.58	
ATOM	3237	СВ	77AL	682		9.433		63.511 62.131		20.10	÷
ATOM	3238	CG1	VAL	682		0.190		60.969		16.40	÷
ATOM	3239		77 L	682		7.952	45.785	61.867		17.19	ě
ATOM	3240	C	7AL	682		8.861		64.001		17.00	÷
MOTA MOTA	3241	0	VAL	682		8.659		63.342		15.10	Ė
ATOM	3242 3243	N CA	LEU LEU	683 683		B.449 7.4 8 5		65.258		17.47	
ATOM	3244	CB	LEU	683		7. 32 6		67.348		20.70	:
MOTA	3245	CG	LEU	683		8.420		68.299	1.00	17.50 13.82	:
ATOM	3246	CD1	-E::	683		8.201		69.667		13.45	:
ATOM	3247		LEU	683		8.376		68.387		15.36	:
MOTA MOTA	3248		LEU	683		6.228		65.104		24.03	:
ATOM	3249 3250	N O	LEU Ser	683 684		5.446 6.087		65.544		24.27	:
ATOM	3251	CA	SER	684		5.003		63.914 63.028	1.00	25.99	
ATOM	3252	CB	SEF.	684		5.222		61.629		26.98 31.20	:
MOTA	3253	OG	SEP.	684		6.502		61.067		36.99	: ;
MOTA	3254	C	SER	684		3.614		63.491		26.69	:
ATOM ATOM	3255 3256	O	IIP.	584		2.800		63.699		27.76	:
ATOM	3256	N CA	ASN ASN	685 685		3.397		63.826		24.94	-
ATOM	3258	CB	AIN	685		2.049 1.716		64.131		25.85	:
ATOM	3259	CG	AEN	685		2.993		63.083 62.504		27.66 28.61	
MOTA	3260	ODI	AE::	685		3.994		62.186		26.41	÷
ATOM	3261		ZEA	685		2.972	38.406	62.407		28.57	-
MOTA MOTA	3262	C	ASN	685		1.748		65.533	1.00	26.76	3
ATOM	3263 3264	Ŋ Ō	AIX LEU	685 686		2.271		€5.923		27.14	÷
ATOM	3265	CA.	LEU	686		0.899 0.583		66.287 67.649		25.95	
ATOM	3266	CB	LEU	686		1.779		68.584		24.26	:
ATOM	3267	CG	LEU	686		2.718		68.474		23.47	
ATOM	3268	CD1	TE::	686	2	3.700		69.708		21.84	-

bref21	.c.pd	b		Thu	Apr	25	12:	:27:	47	1996		,	43	
ATOM	3269	CD2	LEU	68 6		3.5		42.74		57.173 58.375		0 20.		5 5
ATOM	3270	С	LEU	686		9.2		41.56 40.66		58.47B		0 27.		à
ATOM	3271 3272	0	LEU ARG	686 687		9.0	35	42.80	1	68.858		0 25.		7
ATOM ATOM	3273	CA	ARG	687		7.8		43.14		69.636		00 21. 00 21.		5
ATOM	3274	CB	ARG	687		8.1	_	42.90		71.113 71. 74 5		00 18		5
MOTA	3275	CD	ARG ARG	687 687		17.7		40.47		71.410	1.0	00 20	. 25	5
ATOM ATOM	3276 3277	NE	ARG	687		16.8		39.42	26	71.911	1.0		.57	7
ATOM	3278	CZ	ARG	687		16.8		38.18		71.416 70.405		00 24 00 25		5 7
ATOM	3279	NH1		687		17.6 15.9		37.83		71.908		00 23		7
MOTA	3280	NH2 C	ARG ARG	687 687		17.3		44.58		69.517		00 23		ó
MOTA MOTA	3281 3282	ŏ	ARG	687		17.8		45.3	69	68.695		00 24		а 7
ATOM	3283	N	GLY	688		16.4		44.9		70.407		00 23 00 22		6
MOTA	3284	CA	GLY	688 688		15.8		46.6		71.874		00 23		6
atom Atom	3285 3286	0	GLY	688		15.3		45.7		72.726		00 21		8
ATOM	3287	N	ARG	689		15.		47.9		72.154		00 23		7 6
ATOM	3288	CA	ARG	689		15.5		48.5 48.5		73.500 73.902		00 23		6
MOTA	3289	CB	ARG ARG	689 689		13.		49.8		74.581		00 20		6
atom Atom	3290 3291	CD	ARG	689		13.		50.9		73.575		.00 18		6
MOTA	3292	NE	ARG	689		14.		52.2		73.908		.00 1°		7 5
MOTA	3293	CZ	ARG	689		14. 13.		52.8 52.2		75.128 76.250	_	.00 1		7
MOTA	3294 3295		ARG ARG	689 689		14.		54.0		75.213		.00 1		7
MOTA MOTA	3296	С	ARG	689			425	47.9		74.648		.00 2		์ 8
ATOM	3297	0	ARG	689			512	48.5		75.756 74.313		.00 2		7
ATOM	3298		THR THR	690 690			153 053	46.3		75.182		.00 2		6
ATOM ATOM	3299 3300			690			530	44.		74.403	3 1	.00 2		5
MOTA	3301		1 THP.	690			550	44.		73.40		.00 2		8 -ნ
MOTA	3302		2 THR	690			808	43. 46.		75.355 75.66		.00 2		6
MOTA	3303		THR THR	690 690			052	47.		74.84		.00 2		8
ATOM ATOM	3304 3305		ARG	691			653	46.		76. 96		.00 2		7
ATOM	3306			691		20.	920	47.		77.51		.00 2		6 6
ATOM	3307			691			. 908 . 668	47.	426 303	79.05 79.86		.00 2		6
MOTA	3308			691 691			.736	_	597	81.40		.00		6
MOTA MOTA	3309 3310						.360	45.	549	82.24		1.00 2		7
ATOM	331	L C					.6B1		632 612	82.95 82.93		1.00		5 7
ATOM	331		il ARG H2 ARG				.331 .337		775			1.00		7
ATOM ATOM	331 331	-	ARG				.024	46.	269	77.11		1.00		5
ATOM	331		ARG	691	l.		.863		.028			1.00 1.00		8 7
MOTA	331						.157		.781 . 89 3			1.00		5
MOTA	331 331						.237		. 885			1.00		5
MOTA MOTA	331						.31	7 44	. 905	74.10			23.60	5
MOTA	332	0 C	D1 TYP				3.303		.575)1 22	1.00	23.69 23.82	5 6
MOTA			El TY				2.544 2.53		.636			1.00	24.04	5
ATOM ATOM			D2 TY				.75		.345	72.3	25	1.00	24.91	6
ATOM			Z TY	R 69	2	2:	1.77	2 43	.022	_			24.40	
ATOM	332	25 0	H TY				1.02 5.53		.086				27.00	
ATOM							5.77		. 64				21.10) B
ATOM ATOM		-	N TH				6.3B	2 45	.56	77.3			19.16	
ATOM			CA TH				7.71	-	. 98				14.99	
ATOM			CB TH				7.87 6.74		. 98 5. 64				14.05	
ATON ATON			OG1 TH				9.15		5.74				12.2	
ATOM			C TH	R 69	93	2	8.70	3 45	5.07				14.4	
ATO	4 33		O TH				8.45 9.81		3.87 5.66				11.0	
ATO:			n Ph Ca Ph		94 94		0.84		4.96			1.00	15.6	8 6
ATO:		_	CB Pi		94	3	0.83	33 4	5.50	74.4	105		18.1	
NTO	м 33	38	CG P	IE 6	94		9.4		5.68 6.86				19.4	
ATO		39	CD1 PI		94 94		28.74 28.61		6.86 4.67				18.4	_
ATO ATO		40 41	CD2 PI		94 94		27.4		7.03			1.00	19.7	1 5
ATO		42	CE2 P	HE 6	94	:	27.6	17 4	4.8				16.4	
ATO	M 33	343			94		26.9		6.02 5.2				16.7 14.8	
ATC ATC		344 345			94		32.2 32.5		6.3				14.7	15 B
ATC		346			95		33.1		4.2		155		14.2	

bref2	lc.po	db		Thu	Apr 25	12:27:47	1996		44	
ATOM	3347	CA	ALA	695	34.53	2 44.271	76.533	1.00 1	14 50	6
ATOM	3348	СB	ALA	695	34.70		77.959	1.00 1		6
ATOM	3349	С	ALA	695	35.33		75.579	1.00 1		6
ATOM	3350	0	ALA	695	34.73		74.883	1.00 1		ě
ATOM	3351	N	VAL	696	36.66		75.554	1.00 1		7
ATOM	3352	CA	VAL	696	37.47		74.640	1.00 1	8.54	6
ATOM ATOM	3353 3354	CB CG1	VAL	696	37.45		73.198	1.00 1		6
ATOM	3355	CG2	VAL VAL	696 696	37.86 38.33		73.223 72.255	1.00 1		6
ATOM	3356	c	VAL	696	38.92		75.047	1.00 2		6
ATOM	3357	0	VAL	696	39.65		75.637	1.00 1		6 8
ATOM	3358	N	ARG	697	39.32		74.738	1.00 1		7
ATOM	3359	CA	ARG	697	40.67	5 40.563	75.050	1.00 1		6
ATOM	3360	CB	ARG	697	40.59		75.664	1.00 1		6
ATOM	3361	CG	ARG	697	39.77		76.889	1.00 1	.5.40	6
ATOM ATOM	3362 3363	CD NE	ARG ARG	697 697	39.84		77.417	1.00 1		6
ATOM	3364	CZ	ARG	697	39.07 38.72		76.632	1.00 1		7
ATOM	3365	NH1	ARG	697	39.06		77.081 78.309	1.00 1		6
ATOM	3366		ARG	697	38.01		76.318	1.00 2		7
ATOM	3367	C	ARG	697	41.62		73.818	1.00 1		6
ATOM	3368	0	ARG	697	41.18		72.677	1.00 1		8
MOTA	3369	И	ALA	698	42.92	6 40.660	74.077	1.00 1		7
ATOM	3370	CA	ALA	698	43.97	3 40.609	73.057	1.00 1		5
ATOM	3371	CB	ALA	698	44.81		73.146	1.00 1		6
ATOM	3372	c	ALA	698	44.83		73.296	1.00 1		6
ATOM ATOM	3373 3374	o N	ALA ARG	698 699	45.07		74.432	1.00 1		8
ATOM	3375	CA	ARG	699	45.34 46.17		72.234	1.00 1		7
ATOM	3376	СВ	ARG	699	45.22		72.325 72.392	1.00 1		5
ATOM	3377	CG	ARG	699	45.69		71.794	1.00 1		6 6
ATOM	3378	CD	ARG	699	46.73		72.665	1.00 2		6
MOTA	3379	NE	ARG	699	46.91	3 32.910	72.399	1.00 2		ž
MOTA	3380	CZ	ARG	699	46.11		72.895	1.00 2		6
ATOM	3381		ARG	699	45.06		73.672	1.00 2		7
ATOM ATOM	3382 3 38 3	C C	ARG ARG	699	46.44		72.710	1.00-2		7
ATOM	3384	0	ARG	699 699	47.09 46.68		71.094	1.00	9.38	6
ATOM	3385	N	MET	700	48.35		69.991 71.282	1.00 1		8
ATOM	3386	CA	MET	700	49.26		70.140	1.00	8.21 7.21	7 6
ATOM	3387	CB	MET	700	50.72		70.551	1.00	6.01	6
ATOM	3388	CG	MET	700	51.32		70.963	1.00	5.33	5
MOTA	3389	SD	MET	700	52.09		69.678	1.00	9.84	16
MOTA	3390	CE	MET	700	51.36	8 40.792	69.955	1.00	8.49	5
ATOM	3391	C	MET	700	48.87		69.375	1.00	6.64	6
ATOM	3392	0	MET	700	48.60		69.939	1.00	6.32	8
ATOM ATOM	3393 3394	N CA	ALA ALA	701 701	48.84 48.42		68.069	1.00	7.50	7
ATOM	3395	CB	ALA	701	47.60		67.250 66.065	1.00	8.94	6
ATOM	3396	c	ALA	701	49.48		66.779	1.00	7.41 9.12	6
ATOM	3397	Ō	ALA	701	50.67		66.639	1.00	9.86	6 3
ATOM	3398	N	GLU	702	48.98		66.491		0.01	7
MOTA	3399	CA	GLU	702	49.76		65.987	1.00 1		6
ATOM	3400	CB	GLU	702	48.97		66.108	1.00 1		6
ATOM	3401	CG	GLU	702	48.72		67.501	1.00 1	–	6
ATOM ATOM	3402 3403	CD	GLU	702	48.59		67.507	1.00 2		5
ATOM		· OE2	GLU	702 702	47.90 49.23		66.611	1.00 2		8
ATOM	3405	C	GLU	702	50.12		68.377 64.510	1.00 2		9
ATOM	3406	ō	GLU	702	49.56		63.802	1.00 1		6 8
ATOM	3407	N	PRO	703	51.10		64.037	1.00 1		.)
ATOM	3408	CD	PRO	703	51.50		62.625	1.00 1		6
ATOM	3409	ÇA	PRO	703	51.78	3 30.007	64.899	1.00 1		์ ร์
MOTA	3410	CB	PRC	703	51.89	6 28.794	63.999	1.00 1		6
ATOM	3411	CG	PRÇ	703	52.25		62.635	1.00 1	9.35	6
ATOM	3412	Ć	PRO	703	53.15		65.409	1.00 1		5
ATOM ATOM	3413	0	PRC	703	53.80		66.157	1.00 1		9
ATOM	3414 3415	N CA	SER SER	704	53.58		65.002	1.00 1		7
ATOM	3415	CB	SER	704 704	54.87 55.15		65.461	1.00	9.78	5
ATOM	3417	OG	SER	704	55.30		64.798 63.394	1.00	9.23 6.65	·5
ATOM	3418	c	SER	704	54.86		67.003	1.00		ห ร
ATOM	3419	Ö	SER	704	55.62		67.736		12.01	a
ATOM	3420	N	PHE	705	53.93	7 33.229	67.468	1.00	8.75	7
ATOM	3421	CA	PHE	705	53.76		68.857	1.00	3.52	6
ATOM ATOM	3422 3423	CB	PHE	705	53.32		68.988	1.00	5.09	6
ATOM	3423	CD1	PHE PHE	705 705	54.15		68.184	1.00	7.49	15
	~ 7		- 115	.00	53.69	6 36.417	66.957	1.00	8.92	15

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ATOM	3425	CD2	PHE	705		55.446		.284	68.611	1.00 8.54 5
ATOM	3426	CEl		705		54.512		.252	66.163	
ATOM	3427	CE2		705		56.270		.115	67.833	1.00 4.91 5 1.00 5.19 5
MOTA	3428	CZ	PHE	705		55.804		.598 2.591	66.606 69.505	1.00 5.11
MOTA	3429	C	PHE	705 705		52.783 52.257		. 697	68.878	1.00 4.57 1.00 8.69
ATOM	3430	0	PHE	705		52.634		.751	70.809	1.00 8.69 7
MOTA	3431	N CA	GLY	706		51.728		.956	71.622	1.00 7.99
atom Atom	3432 3433	C	GLY	706		51.661	32	2.726	72.932	1.00 9.39
ATOM	3434	Ö	GLY	706		52.345	33	3.739	73.069	1.00 9.05
ATOM	3435	N	GLY	707		50.829		2.295	73.878	1.00 10.91 7 1.00 9.87 5
ATOM	3436	CA	GLY	707		50.738		2.990	75.162	
ATOM	3437	С	GLY	707		49.465		2.823	75.977 76.063	1.00 7.80 5 1.00 7.37 3
ATOM	3438	0	GLY	707		48.894		1.731 3.927	76.540	1.00 7.59 7
ATOM	3439	N CA	PHE	708 708		47.801		3.911	77.372	1.00 8.42 5
ATOM	3440 3441	CB	PHE	708		48.171		3.981	78.874	1.00 9.14 5
MOTA MOTA	3442	CG	PHE	708		49.358	3	3.126	79.277	1.00 8.19 5
ATOM	3443		PHE	708		49.19		1.787	79.592	1.00 5.98 5
ATOM	3444		PHE	708		50.638		3.679	79.352	1.00 6.32 ÷ 1.00 8.74 ÷
MOTA	3445		PHE	708		50.29		1.016	79.974 79.731	1.00 5.05
ATOM	3446		PHE	708		51.73		1.587	80.040	
ATOM	3447	cz	PHE	708 708		46.84		5.066	77.077	1.00 7.99 5
ATOM	3448	0	PHE	708		47.26		6.187	76.721	1.00 6.94 =
ATOM	3449 3450	N	TRP	709		45.56		34.777	77.285	1.00 9.09 7
ATOM ATOM	3451	CA	TRP	709		44.47	5 3	35.752	77.119	
ATOM	3452	СВ	TRP	709		43.11		35.083	77.396	1.00 11.59
ATOM	3453	CG	TRP	709		42.41		34.592	76.165	
ATOM	3454		2 TRP	709		42.09		35.354	74.999	
MOTA	3455	CE		709		41.46		34.481 36 687	74.092	
MOTA	3456					42.28		36.687 33.326		
ATOM	3457		1 TRP			41.39		33.250		·
MOTA	3458		1 TRE			41.01		34.897		1 1.00 9.03 5
ATOM	3459 3460		3 TRE			41.83		37.103		9 1.00 11.59 5
MOTA MOTA	3461					41.2		36.209		
ATOM	3462		TRE		•	44.6		36.973		
ATOM	3463		TRI			44.7		36.823		
ATOM	3464		SE			44.6		38.177		
MOTA	3465					44.7		39.350		
MOTA	3466			_		43.8		41.25		7 1.00 10.05 3
MOTA MOTA	3461 3461		SE			43.5		39.56		6 1.00 12.22 5
ATOM	346		SE			42.5	31	38.83		
ATOM	347			_	1	43.5	80	40.56		6 1.00 12.01
ATOM	347		A AL	A 71	7	42.4		40.86		
ATOM	347	2 C				42.8		41.81		
ATOM						41.4		41.56		
ATOM			_	_		41.8		41.55		
ATOM			TR A TP			39.1		42.25		27 1.00 12.59 f
MOTA MOTA			B TF			37.7		42.03		92 1.00 8.73 ÷
ATOM	_		G TF			37.2	202	40.64		45 1.00 8.57 -
ATOM			D2 TF			36.		40.09		_
ATOM			E2 TI		12	36.		38.74		
MOTA	348		E3 Ti		12	36. 37.		40.60		
MOTA			D1 T	1 PD 7	12 12	36.		38.49		
1OTA 1OTA			CZ2 T		12	35.		37.9		83 1.00 8.46
ATON			23 T		12	36.		39.7		
ATO			CH2 T		12	35.		38.4		
ATO			C T		12		498	43.7		
ATO	4 341	88 (12		124	44.2	_	
ATO				_	13		174 366	44.3 45.8		
ATO					13		294	45.0		
ATO					13		973	45.8		149 1.30 11.86
ATO ATO					13		167	46.4		799 1.00 15.88
ATO					13		081	45.9		764 1.00 18.64
ATO					114		309			
ATO				LU	114		. 163			888 1.00 20.29
ATO	M 34	97			114		. 524			27600 21.54
ATC		98			714		470			
ATC		199			714		.699 .860			420 1.00 27.51
ATC		500 501	OE1 (714 714		.735			957 1.00 25.69
ATC ATC		502			714		.885			027 1.00 21.46

bref2	1c.po	I b		Thu	Apr	25	12:27:47	1996		46	
ATOM	3503	0	GLU	714	3	5.86	7 48.844	77.886	1.00	21.24	а
ATOM	3504	N	PRO	715	3	4.78	7 47.852	79.611		20.46	7
ATOM	3505	CD	PRO	715	3	4.70	3 47.767	81.090	1.00	21.13	5
ATOM	3506	CA	PRO	715	3	3.46	0 47.694	79.015		19.23	5
ATOM	3507	CB	PRO	715	3	2.62	7 47.183	80.182		21.32	5
MOTA	3508	CG	PRO	715	3	3.22	6 47.974	81.352		19.98	5
ATOM	3509	С	PRO	715		2.87		78.473		20.02	5
ATOM	3510	0	PRO	715	3	3.19	4 50.060	78.922		20.10	à
ATOM	3511	N	VAL	716		1.93		77.562	1.00	20.51	7
ATOM	3512	CA	VAL	716	3	1.22	9 49.858	76.910	1.00	19.79	5
ATOM	3513	CB	VAL	716		1.76		75.440	1.00	18.56	5
MOTA	3514	CG1		716		0.98		74.396	1.00	18.80	5
ATOM	3515	CG2	VAL	716		1.74		75.099	1.00	16.95	ó
ATOM	3516	С	VAL	716		9.77		76. 9 08	1.00	21.79	5
MOTA	3517	0	VAL	716	2	9.51	5 48.182	76.624	1.00	20.72	8
MOTA	3518	N	SER	717	2	8.85	9 50.269	77.264	1.00	22.27	7
ATOM	3519	CA	SER	717		7.43		77.331		21.09	6
ATOM	3520	CB	SER	717		6.92		78.764	1.00	23.89	5
ATOM	3521	OG	SER	717		7.18		79.607	1.00	24.17	8
MOTA	3522	С	SER	717		6.55		76.375	1.00	20.65	6
ATOM	3523	0	SER	717		6.54		76.394	1.00	19.78	8
ATOM	3524	N	LEU	718		5.83		75.523	1.00	21.29	7
MOTA	3525	CA	LEU	718		4.B6		74.585		21.71	5
ATOM	3526	CB	LEU	718		5.00		73.188	1.00	17.72	5
ATOM	3527	CG	LEU	718		4.50		72.057		15.29	5
ATOM	3528		LEU	718		5.27		72.069	1.00	11.08	6
MOTA	3529		LEU	718		4.63		70 .73 3		11.73	ó
ATOM	3530	C	LEU	718		3.47		75.183		22.58	5
ATOM	3531	0	LEU	718		3.39		76.191		24.55	3
ATOM	3532	N	LEU	719		2.39		74.564		23.55	7
ATOM	3533	CA	LEU	719		1.02		75.054		23.37	5
MOTA	3534	CB	LEU	719		0.63		76.069		23.00	6
ATOM	3535	CG	LEU	719		1.54		77.325		22.19	5
ATOM	3536		LEU	719		1.29		78.084		19.79	5
ATOM	3537		LEU	719		1.41		78.254		20.88	6
ATOM	3538	C	LEU	719		9.98		73.904		23.18	6
ATOM	3539	0	LEU	719		8.88		74.036		24.17	8
MOTA	3540	N	THR	720		0.32		72.828		22.42	7
ATOM	3541	CA	THP.	720		9.49		71.597		21.89	£
MOTA	3542	CB	THR	720		9.03		71.295		22.47	Ó
MOTA	3543	0G1	THE	720		B.79		72.513		24.25	8
ATOM	3544	CG2		720		0.04		70.444		20.74	5
MOTA	3545	C	THE	720		8.26		71.492		22.94	5
MOTA	3546	0	THP.	720	1	7.14	10 49.947	71.240	1.00	22.69	ð

Table										
Data Set	Resolution	Reflections	Completeness	R _{sym} S	Sites R _{iso}		Roullis	RKraut	Phasing Power's	Powers
0 iii	(Å) 25.0-2.8	(#) 14158	0.93(0.91)	0.05	1	t	•	1	ı	•
HgAC ₂	25.0-3.0	11496	0.93 (0.91)	0.10	7	0.102	0.56	0.114	IBO 1.87 (3.1Å) Ano 1.35 (4.0Å)	(3.1Å) (4.0Å)
UO2 (NO3)2	25.0-3.0	11931	0.96 (0.94)	0.14	4	0.116	0.62	0.137	Iso 1.95 (3.1Å) Ano 1.72 (3.9Å)	(3.1Å) (3.9Å)
	4 6			RMS from ideal values	m idea	l value	60	Average	Average B Value (Å ²)	(Ų)
Refinement	Refinement Statistics.				4	elong boom	9100	EBP1	EBP2	Peptides
Resolution (Å)	Resolution Relflections Total R (Å) F>10 of a	Total Number of atoms	R-value	Bond Length	5		, , , , , , , , , , , , , , , , , , ,			
	7000	3462	0.21		0.016	0.016(Å)	2.1	10.5	10.5 12.3	10.7
8.0-2.8	1 1874	1	!	•						

 $*R_{sym} = E | I - < I > /E I$.

tRiso=El FpH-Fp /EFp.

TR (FPH(obs) FPH(calc) | F PH(obs) F PH(calc) | / [F PH(obs) F PH(obs) for all acentric relfections (anamalous case). $^{\dagger}R_{Cullis}$ = Σ | F_{PH} + F_P | - $F_{H(calc)}$ | / F_{PH} - F_P | for all centric reflections.

SPhase Power={[Streater] 2/2 FpH(obs) Fp(cate) 2 1/2 1 FpH(obs) Fp(cate) is the lack of closure error to maximum resolution indicated. Hean Figure of Merit=<| $P(\alpha)e^{i\alpha}/LP(\alpha)|$ > where $P(\alpha)$ is the phase probability.

 a Completeness of data in the outer shell, (2.9-2.8Å) for the native and (3.1-3.0Å) for both derivatives.

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Peptidel-EBP1	Peptidel-EBP2	Peptidel-EBP2	Peptide2-EBP1	Peptide2-EBP1 Peptide1-Peptide2
Gly ^{P9} O-Met ¹⁵⁰ N	Tyr ^{P4} OH-Ser ⁹² N	Gly ^{P9} O-Met ¹⁵⁰ N	Tyr ^{P4} OH-Ser ⁹² N Tyr ^{P4} O-Cys ^{P6} N	Tyr ^{P4} 0-cy8 ^{P6} N
Pro ^{P10} 0-Thr ¹⁵¹ N		Pro ^{P10} 0-Thr ¹⁵¹ N		Tyr P4N-CysP6O
Pro ^{P10} 0-Thr ¹⁵¹ 0γ		$Pro^{P10}O-Thr^{151}O\gamma 1$		Cys ^{P6} O-Tyr ^{P4} N
Leu ^{P11} 0-Ser ¹⁵² N		Leu ^{P11} 0-Ser ¹⁵² N		Cys ^{P6} N-Tyr ^{P4} O
Leu ^{P11} 0-Ser ¹⁵² 07		Leu ^{P11} 0-Ser ¹⁵² 0y		

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CLAIMS

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What is claimed is:

- 1. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
 - (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
 - (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
 - (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
 - (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.

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- 2. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
 - (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is cocrystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
 - (b) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said criteria data set;
 - (c) outputting to said output device the constructed model.
- 3. A compound having a chemical structure selected using the method of claim 1, said compound being an EPO mimetic.
 - 4. The compound of claim 3 wherein said compound is not a peptide.
 - 5. The compound of claim 3 wherein said compound is a peptide.
 - 6. The compound of claims 5 wherein said peptide has 15 of fewer amino acids.

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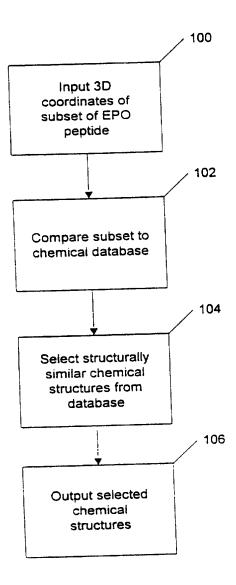


FIG. 1

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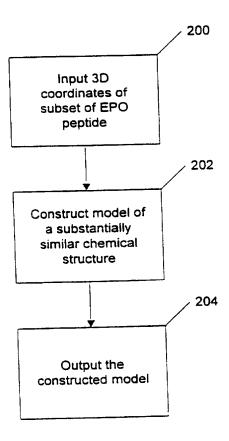


FIG. 2

INTERNATIONAL SEARCH REPORT

International application No. PCT/US97/07218

	TO STONE OF COMPECT MATTER		
	SIFICATION OF SUBJECT MATTER G06F 159:00		
TIC CI .2	1641406	IDO	
According to	International Patent Classification (IPC) or to both na	tional classification and IPC	
B. FIELI	DS SEARCHED	1 (5 - A)	
Minimum do	cumentation searched (classification system followed b	y classification symbols)	
U.S. : 3	64/496, 497,498,578		
	on searched other than minimum documentation to the e	extent that such documents are included i	n the fields searched
Documentati	on searched other than minimum documentation to also		
Electronic da	ata base consulted during the international search (nam	e of data base and, where practicable,	search terms used)
aps, dialo			
search te	rms: erythropoietin, receptor, 3d, pdb or databa	se	
C. DOC	UMENTS CONSIDERED TO BE RELEVANT		
Category*	Citation of document, with indication, where app	ropriate, of the relevant passages	Relevant to claim No.
	US, 5,331,573 A (BALAJI et al.) 19	July 1994 (col. 7, lines	1-6
X	46-66, col. 13, lines 20-55, col. 14	1 lines 12-23	
	40-00, COI. 13, lines 20-33, COI. 1-	.,	
A,P	US 5,557,535 A (SRINIVASAN et	al.) 17 September 1996,	1,2
	(abstract, fig. 1, col. 4, line 57 - co	ol. 6,line 55)	
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	fig. 8, fig. 12)		
		22 November 1993 (CO	1,2
Α	US 5,265,030 A (SKOLNICK et al.)	23 November 1993, (co.	1,2
	2, line 20 - col. 3, line 20)		
A D	MCCARTHY, "Small Peptide De	signed that can Mimic	1-6
A,P	Erythropoietin" Lancet, 8/96 vol.	348, no. 24, p.395	
	Livinopolotiii Landay eras		
X Furt	her documents are listed in the continuation of Box C.	. See patent family annex.	
• s	pecial categories of cited documents:	"T" later document published after the indate and not in conflict with the appli	ternational filing date or priority cation but cited to understand the
.v. q	ocument defining the general state of the art which is not considered to be part of particular relevance	principle or theory underlying the in	vention
L	arlier document published on or after the international filing date	"X" document of particular relevance; to considered novel or cannot be considered.	he claimed invention cannot be ered to involve an inventive step
a	ocument which may throw doubts on priority claim(s) or which is ited to establish the publication date of another citation or other	when the document is taken alone	
-	pecial reason (as specified)	"Y" document of particular relevance; to considered to involve an inventive combined with one or more other su	e aten when the document is
	ocument referring to an oral disclosure, use, exhibition or other neans	combined with one or more other su being obvious to a person skilled in	the art
·P· d	ocument published prior to the international filing date but later than	*&* document member of the same peter	at family
	he priority date claimed e actual completion of the international search	Date of mailing of the international se	earch report
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Name and	mailing address of the ISA/US	Authorized officer	
Box PCT		MELANIE KEMPER	
1	on, D.C. 20231 No. (703) 305-3230	Telephone No. (703) 305-3900	

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US97/07218

Category*	citation of documents with the citation of the citat	T T
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No
ζ,P	LIVNAH ET AL., "Functional Mimicry of a Protein Hormone by a Peptide Agonist" Science 26 July 1996, vol. 273 no. 274, p. 464-471.	1-6